d his ful

(FILE 'HOME' ENTERED AT 17:20:35 ON 31 AUG 2005)

FILE 'REGISTRY' ENTERED AT 17:20:39 ON 31 AUG 2005
L1   STRUCTURE UPLOADED
L2   17 SEA SSS FUL L1
           D L2 1-17 ED

FILE 'HCAPLUS' ENTERED AT 17:21:29 ON 31 AUG 2005
L3   3 SEA PLU=ON   L2
           D L3 1-3 IBIB

FILE 'REGISTRY' ENTERED AT 17:46:40 ON 31 AUG 2005
L4   STRUCTURE UPLOADED
L5   20 SEA SSS FUL L4

FILE 'HCAPLUS' ENTERED AT 17:47:06 ON 31 AUG 2005
L6   1 SEA PLU=ON   L5
            D L6

FILE HOME

FILE REGISTRY
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STRUCTURE FILE UPDATES: 30 AUG 2005   HIGHEST RN 862155-39-3
DICTIONARY FILE UPDATES: 30 AUG 2005   HIGHEST RN 862155-39-3

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  ****
  *   *
  * The CA roles and document type information have been removed from *
  * the IDE default display format and the ED field has been added,   *
  * effective March 20, 2005. A new display format, IDERL, is now   *
  * available and contains the CA role and document type information. *
  *   *
  ****

  Structure search iteration limits have been increased. See HELP SLIMITS
  for details.

  Experimental and calculated property data are now available. For more
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  to the file summary sheet on the web at:
  http://www.cas.org/ONLINE/DBSS/registryss.html

FILE HCAPLUS

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FILE COVERS 1907 - 31 Aug 2005   VOL 143 ISS 10
FILE LAST UPDATED: 30 Aug 2005   (20050830/ED)

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 This file contains CAS Registry Numbers for easy and accurate
 substance identification.

```
=> d his ful

     (FILE 'HOME' ENTERED AT 14:21:20 ON 31 AUG 2005)

     FILE 'REGISTRY' ENTERED AT 14:21:26 ON 31 AUG 2005
L1              STRUCTURE UPLOADED
L2          50 SEA SSS SAM L1
L3        2305 SEA SSS FUL L1
L4              STRUCTURE UPLOADED
L5        2199 SEA SUB=L3 SSS FUL L4
L6              STRUCTURE UPLOADED
L7        2199 SEA SUB=L5 SSS FUL L6
L8              STRUCTURE UPLOADED
L9        2107 SEA SUB=L7 SSS FUL L8
L10         92 SEA PLU=ON  L7 NOT L9

     FILE 'HCAPLUS, USPATFULL, TOXCENTER' ENTERED AT 14:28:20 ON 31 AUG 2005
L11        281 SEA PLU=ON  L10
L12        259 DUP REM L11 (22 DUPLICATES REMOVED)
                   ANSWERS '1-237' FROM FILE HCAPLUS
                   ANSWERS '238-259' FROM FILE USPATFULL

     FILE 'HCAPLUS, USPATFULL' ENTERED AT 14:28:56 ON 31 AUG 2005
L13        259 SEA PLU=ON  L12
L14        253 SEA PLU=ON  L13 AND (PD<20030129 OR PRD<20030129)
L15        243 SEA PLU=ON  L14 AND PD<20020129
L16        243 DUP REM L15 (0 DUPLICATES REMOVED)
                   ANSWERS '1-225' FROM FILE HCAPLUS
                   ANSWERS '226-243' FROM FILE USPATFULL
               D L16 226-243 IBIB HITSTR

     FILE 'REGISTRY' ENTERED AT 14:35:10 ON 31 AUG 2005
L17             STRUCTURE UPLOADED
L18        359 SEA SUB=L9 SSS FUL L17
L19             STRUCTURE UPLOADED
               D L1
L20       1151 SEA SUB=L3 SSS FUL L19
               D QUE STA
L21       1151 SEA SUB=L20 SSS FUL L4
L22             STRUCTURE UPLOADED
L23        232 SEA SUB=L20 SSS FUL L22

     FILE 'HCAPLUS, USPATFULL' ENTERED AT 14:42:34 ON 31 AUG 2005
L24        136 SEA PLU=ON  L23
L25        113 SEA PLU=ON  L24 AND (PD<20030129 OR PRD<20030129)
L26        108 DUP REM L25 (5 DUPLICATES REMOVED)
                   ANSWERS '1-81' FROM FILE HCAPLUS
                   ANSWERS '82-108' FROM FILE USPATFULL

     FILE 'REGISTRY' ENTERED AT 14:44:13 ON 31 AUG 2005
L27             STRUCTURE UPLOADED
L28         43 SEA SUB=L23 SSS FUL L27
               D QUE STA

     FILE 'HCAPLUS, USPATFULL' ENTERED AT 14:45:45 ON 31 AUG 2005
L29         15 SEA PLU=ON  L28
L30         14 SEA PLU=ON  L28 AND (PD<20030129 OR PRD<20030129)
L31         13 DUP REM L30 (1 DUPLICATE REMOVED)
                   ANSWERS '1-9' FROM FILE HCAPLUS
                   ANSWERS '10-13' FROM FILE USPATFULL
L32         13 SEA PLU=ON  L31 AND L26
               D QUE STA
               D L32 1-13 IBIB HITSTR
```

FILE HOME

FILE REGISTRY
Property values tagged with IC are from the ZIC/VINITI data file
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STRUCTURE FILE UPDATES: 30 AUG 2005   HIGHEST RN 862155-39-3
DICTIONARY FILE UPDATES: 30 AUG 2005   HIGHEST RN 862155-39-3

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TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

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****
*   *
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*   *
****

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http://www.cas.org/ONLINE/DBSS/registryss.html

FILE HCAPLUS
FILE COVERS 1907 - 31 Aug 2005   VOL 143 ISS 10
FILE LAST UPDATED: 30 Aug 2005   (20050830/ED)

FILE USPATFULL
FILE COVERS 1971 TO PATENT PUBLICATION DATE: 30 Aug 2005 (20050830/PD)
FILE LAST UPDATED: 30 Aug 2005 (20050830/ED)
CA INDEXING IS CURRENT THROUGH 30 Aug 2005 (20050830/UPCA)
ISSUE CLASS FIELDS (/INCL) CURRENT THROUGH: 30 Aug 2005 (20050830/PD)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Jun 2005

FILE TOXCENTER
FILE COVERS 1907 TO 30 Aug 2005 (20050830/ED)

```
=> d his ful

      (FILE 'REGISTRY' ENTERED AT 15:38:28 ON 31 AUG 2005)
                  DEL HIS
L1                STRUCTURE UPLOADED
L2                STRUCTURE UPLOADED
L3          2305 SEA SSS FUL L2
L4             0 SEA SUB=L3 SSS FUL L1
L5                STRUCTURE UPLOADED
L6             0 SEA SSS FUL L5
L7                STRUCTURE UPLOADED
L8             2 SEA SSS SAM L7
L9            30 SEA SSS FUL L7


      FILE 'HCAPLUS, USPATFULL' ENTERED AT 15:48:07 ON 31 AUG 2005
L10            5 SEA PLU=ON  L9
L11            5 DUP REM L10 (0 DUPLICATES REMOVED)
                  ANSWERS '1-3' FROM FILE HCAPLUS
                  ANSWERS '4-5' FROM FILE USPATFULL
              D L11 1-5 IBIB HITSTR


      FILE 'MARPAT' ENTERED AT 15:49:26 ON 31 AUG 2005


      FILE 'REGISTRY' ENTERED AT 15:58:38 ON 31 AUG 2005
L12               STRUCTURE UPLOADED
L13           10 SEA SSS FUL L12


      FILE 'HCAPLUS, USPATFULL' ENTERED AT 15:59:29 ON 31 AUG 2005
L14            4 SEA PLU=ON  L13
L*** DEL       4 DUP REM L14 (0 DUPLICATES REMOVED)
                  ANSWERS '1-2' FROM FILE HCAPLUS
                  ANSWERS '3-4' FROM FILE USPATFULL
              D L14 1-4 IBIB HITSTR
L15               STRUCTURE UPLOADED


      FILE 'REGISTRY' ENTERED AT 16:04:53 ON 31 AUG 2005
L16           34 SEA SSS FUL L15


      FILE 'HCAPLUS' ENTERED AT 16:04:58 ON 31 AUG 2005
L17            5 SEA PLU=ON  L16
              D L17 1-5 CBIB
              D L17 1-5 IBIB HITSTR


      FILE 'REGISTRY' ENTERED AT 16:13:56 ON 31 AUG 2005
L18               STRUCTURE UPLOADED
L19               STRUCTURE UPLOADED
L20               STRUCTURE UPLOADED
L21               STRUCTURE UPLOADED
L22            6 SEA SSS FUL L18
L23           10 SEA SSS FUL L19
L24            2 SEA SSS FUL L20
L25            0 SEA SSS FUL L21
L*** DEL      18 L22 OR L23 OR L24


      FILE 'HCAPLUS' ENTERED AT 16:18:30 ON 31 AUG 2005
L26           10 SEA PLU=ON  L22 OR L23 OR L24
L27           10 DUP REM L26 (0 DUPLICATES REMOVED)
                  ANSWERS '1-10' FROM FILE HCAPLUS
L28           10 SEA L27
L29            3 SEA L11
L30           10 SEA PLU=ON  L28 NOT L29 OR L14
              D L30 1-10 IBIB HITSTR


      FILE 'STNGUIDE' ENTERED AT 16:22:17 ON 31 AUG 2005
```

```
        FILE 'CASREACT' ENTERED AT 16:23:20 ON 31 AUG 2005
L31              0 SEA PLU=ON  L22
L32              0 SEA SSS SAM L18 (     0 REACTIONS)
L33              0 SEA SSS FUL L18 (     0 REACTIONS)
L34              0 SEA SSS FUL L19 (     0 REACTIONS)
L35              1 SEA SSS FUL L20 (     1 REACTIONS)
                 D L35 CBIB
L36              0 SEA PLU=ON  L23
                 D L35 HITRXN
L37              0 SEA SSS FUL L15 (     0 REACTIONS)
L38              0 SEA SSS FUL L12 (     0 REACTIONS)
```

FILE HCAPLUS
FILE COVERS 1907 - 31 Aug 2005   VOL 143 ISS 10
FILE LAST UPDATED: 30 Aug 2005   (20050830/ED)

FILE USPATFULL
FILE COVERS 1971 TO PATENT PUBLICATION DATE: 30 Aug 2005 (20050830/PD)
FILE LAST UPDATED: 30 Aug 2005 (20050830/ED)
CA INDEXING IS CURRENT THROUGH 30 Aug 2005 (20050830/UPCA)
ISSUE CLASS FIELDS (/INCL) CURRENT THROUGH: 30 Aug 2005 (20050830/PD)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Jun 2005

FILE MARPAT
FILE CONTENT: 1988-PRESENT (VOL 143 ISS 09)(20050826/ED)

MOST RECENT CITATIONS FOR PATENTS FROM FIVE MAJOR ISSUING AGENCIES
(COVERAGE TO THESE DATES IS NOT COMPLETE):

US   6903214 07 JUN 2005
DE   10350965 25 MAY 2005
EP   1538192 08 JUN 2005
JP 2005136379 26 MAY 2005
WO 2005060437 07 JUL 2005

Expanded G-group definition display now available.

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DICTIONARY FILE UPDATES: 30 AUG 2005 HIGHEST RN 862155-39-3

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```
******************************************************************
*                                                                *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added,  *
* effective March 20, 2005.  A new display format, IDERL, is now   *
* available and contains the CA role and document type information. *
*                                                                *
******************************************************************
```

Structure search iteration limits have been increased. See HELP SLIMITS
for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
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FILE CONTAINS CURRENT INFORMATION.
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FILE CONTENT:1840 - 28 Aug 2005 VOL 143 ISS 9

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```
*********************************************************
*                                                       *
*      CASREACT now has more than 9.2 million reactions  *
*                                                       *
*********************************************************
```

Some CASREACT records are derived from the ZIC/VINITI database (1974-1991)
provided by InfoChem, INPI data prior to 1986, and Biotransformations
database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance
identification.

```
> d his ful

     (FILE 'HOME' ENTERED AT 17:20:35 ON 31 AUG 2005)

     FILE 'REGISTRY' ENTERED AT 17:20:39 ON 31 AUG 2005
L1              STRUCTURE UPLOADED
L2        17 SEA SSS FUL L1
                D L2 1-17 ED

     FILE 'HCAPLUS' ENTERED AT 17:21:29 ON 31 AUG 2005
L3         3 SEA PLU=ON   L2
                D L3 1-3 IBIB

     FILE 'REGISTRY' ENTERED AT 17:46:40 ON 31 AUG 2005
L4              STRUCTURE UPLOADED
L5        20 SEA SSS FUL L4

     FILE 'HCAPLUS' ENTERED AT 17:47:06 ON 31 AUG 2005
L6         1 SEA PLU=ON   L5
                D L6
L7              STRUCTURE UPLOADED
                D L7
                S L7

     FILE 'REGISTRY' ENTERED AT 18:34:56 ON 31 AUG 2005
L8         3 SEA SSS SAM L7

     FILE 'HCAPLUS' ENTERED AT 18:34:57 ON 31 AUG 2005
L9         4 SEA PLU=ON   L8
                D L9

     FILE 'CASREACT' ENTERED AT 18:35:15 ON 31 AUG 2005
L10        0 SEA SSS SAM L7 (      0 REACTIONS)
L11      105 SEA SSS FUL L7 (    920 REACTIONS)

     FILE 'REGISTRY' ENTERED AT 18:36:57 ON 31 AUG 2005
                D L8
                D L8 2-3
L12             STRUCTURE UPLOADED
L13     1922 SEA SSS FUL L12
L14             STRUCTURE UPLOADED
L15       13 SEA SUB=L13 SSS FUL L14

     FILE 'HCAPLUS' ENTERED AT 18:44:43 ON 31 AUG 2005
L16        6 SEA PLU=ON   L15

     FILE 'CASREACT' ENTERED AT 18:45:00 ON 31 AUG 2005
L17        0 SEA PLU=ON   L15
L18        0 SEA SSS SAM L14 (      0 REACTIONS)
L19        0 SEA SSS FUL L14 (      0 REACTIONS)

     FILE 'HCAPLUS' ENTERED AT 18:45:34 ON 31 AUG 2005
                D L16 1-6 IBIB HITSTR

     FILE 'STNGUIDE' ENTERED AT 18:47:07 ON 31 AUG 2005

     FILE 'HCAPLUS' ENTERED AT 18:49:08 ON 31 AUG 2005
                SET LINE 250
                SET DETAIL OFF
                E "146474-01-3"/BI,RN 25
                SET NOTICE 1000 SEARCH
L20        2 SEA PLU=ON   146474-01-3/BI
L21        2 SEA PLU=ON   146474-01-3/BI
                SET NOTICE OFF DISPLAY
```

```
              SET LINE LOGIN
              SET DETAIL LOGIN
              DIS L21 1 HIT
              DIS L21 2 HIT
              DIS L21 1 IBIB
              DIS L21 2 IBIB
              SET NOTICE LOGIN DISPLAY
              SET NOTICE LOGIN SEARCH

       FILE 'REGISTRY' ENTERED AT 18:55:05 ON 31 AUG 2005
L22            STRUCTURE UPLOADED
L23         248 SEA SUB=L13 SSS FUL L22

       FILE 'HCAPLUS' ENTERED AT 18:56:00 ON 31 AUG 2005
L24         180 SEA PLU=ON  L23
L25         138 SEA PLU=ON  L24 AND PD<20030129
L26          80 SEA PLU=ON  L24 AND PRD<20030129
L27         122 SEA PLU=ON  L24 AND PD<20020129
              D L27 1-5 IBIB HITSTR

       FILE 'STNGUIDE' ENTERED AT 18:58:14 ON 31 AUG 2005

       FILE 'HCAPLUS' ENTERED AT 19:00:41 ON 31 AUG 2005

       FILE 'STNGUIDE' ENTERED AT 19:05:31 ON 31 AUG 2005

       FILE 'HCAPLUS' ENTERED AT 19:09:34 ON 31 AUG 2005
              D L27 110-122 IBIB HITSTR

       FILE 'STNGUIDE' ENTERED AT 19:09:36 ON 31 AUG 2005

       FILE 'HCAPLUS' ENTERED AT 19:16:25 ON 31 AUG 2005
              D L27 100-109 IBIB HITSTR

       FILE 'STNGUIDE' ENTERED AT 19:16:28 ON 31 AUG 2005

       FILE 'HCAPLUS' ENTERED AT 19:17:26 ON 31 AUG 2005

       FILE 'HCAPLUS' ENTERED AT 19:17:27 ON 31 AUG 2005
L28          13 SEA PLU=ON  L27 AND FLUORO?
              D L28 1-13 IBIB HITSTR KWIC

       FILE 'STNGUIDE' ENTERED AT 19:18:27 ON 31 AUG 2005


       FILE HOME

       FILE REGISTRY
       Property values tagged with IC are from the ZIC/VINITI data file
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       STRUCTURE FILE UPDATES:   30 AUG 2005  HIGHEST RN 862155-39-3
       DICTIONARY FILE UPDATES:  30 AUG 2005  HIGHEST RN 862155-39-3

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       **********************************************************
       *                                                        *
       * The CA roles and document type information have been removed from *
```

```
*  the IDE default display format and the ED field has been added,   *
*  effective March 20, 2005.  A new display format, IDERL, is now     *
*  available and contains the CA role and document type information.  *
*                                                                     *
*********************************************************************

Structure search iteration limits have been increased.  See HELP SLIMITS
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FILE LAST UPDATED: 30 Aug 2005  (20050830/ED)

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*                                                           *
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*                                                           *
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This file contains CAS Registry Numbers for easy and accurate substance
identification.

FILE STNGUIDE
FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Aug 26, 2005 (20050826/UP).

=> d que sta
L12                STR
```
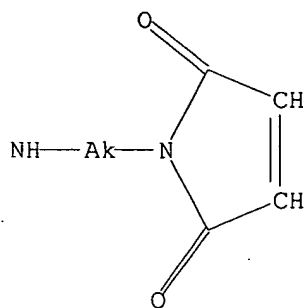
Structure attributes must be viewed using STN Express query preparation.
L13   1922 SEA FILE=REGISTRY SSS FUL L12
L22   STR
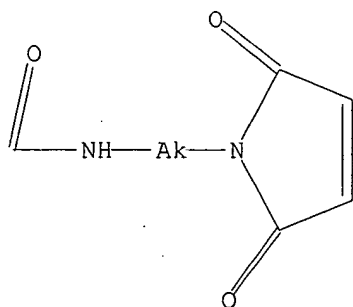
Structure attributes must be viewed using STN Express query preparation.
L23   248 SEA FILE=REGISTRY SUB=L13 SSS FUL L22
L24   180 SEA FILE=HCAPLUS PLU=ON L23
L27   122 SEA FILE=HCAPLUS PLU=ON L24 AND PD<20020129
L28   13 SEA FILE=HCAPLUS PLU=ON L27 AND FLUORO?

```
chain nodes :
    10   11   12   14   16   27   28   29   31   32   33   34   35   36   37   38   39   40   41
    45   46
ring nodes :
    1    2    3    4    5    6    7    8    9    18   19   20   21   22   23   24   25   26   42   43   44
    47   48   49
chain bonds :
    3-16   8-32   9-14   10-11   11-12   14-29   20-28   25-32   26-27   27-31   33-34
    34-35   35-36   36-37   37-38   38-39   40-41   41-42   44-45   45-46
ring bonds :
    1-2   1-6   2-3   3-4   4-5   5-6   5-7   6-9   7-8   8-9   18-19   18-23   19-20
    20-21   21-22   22-23   22-24   23-26   24-25   25-26   42-43   42-47   43-44   44-49
    47-48   48-49
exact/norm bonds :
    1-2   1-6   2-3   3-4   3-16   4-5   5-6   5-7   6-9   7-8   8-9   8-32   9-14   10-11
    11-12   14-29   18-19   18-23   19-20   20-21   20-28   21-22   22-23   22-24   23-26
    24-25   25-26   25-32   26-27   27-31   33-34   34-35   35-36   36-37   37-38   38-39
    40-41   41-42   42-43   42-47   43-44   44-45   44-49   45-46   47-48   48-49
```

G1:H,SO3H

G2:O,S,[*1]

G3:[*2-*3],[*4-*5]

```
Match level :
    1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   6:Atom   7:Atom   8:Atom   9:Atom
    10:CLASS   11:CLASS   12:CLASS   14:CLASS   16:CLASS   18:Atom   19:Atom   20:Atom
    21:Atom   22:Atom   23:Atom   24:Atom   25:Atom   26:Atom   27:CLASS   28:CLASS
    29:CLASS   31:CLASS   32:CLASS   33:CLASS   34:CLASS   35:CLASS   36:CLASS
    37:CLASS   38:CLASS   39:CLASS   40:CLASS   41:CLASS   42:Atom   43:Atom   44:Atom
    45:CLASS   46:CLASS   47:Atom   48:Atom   49:Atom
```

chain nodes :
    10   11   12   14   16   27   28   29   31   32   33   34   35   36   37   38   39   40   41
    45   46
ring nodes :
    1   2   3   4   5   6   7   8   9   18   19   20   21   22   23   24   25   26   42   43   44
    47   48   49
chain bonds :
    3-16   8-32   9-14   10-11   11-12   14-29   20-28   25-32   26-27   27-31   33-34
    34-35   35-36   36-37   37-38   38-39   40-41   41-42   44-45   45-46
ring bonds :
    1-2   1-6   2-3   3-4   4-5   5-6   5-7   6-9   7-8   8-9   18-19   18-23   19-20
    20-21   21-22   22-23   22-24   23-26   24-25   25-26   42-43   42-47   43-44   44-49
    47-48   48-49
exact/norm bonds :
    1-2   1-6   2-3   3-4   3-16   4-5   5-6   5-7   6-9   7-8   8-9   8-32   9-14   10-11
    11-12   14-29   18-19   18-23   19-20   20-21   20-28   21-22   22-23   22-24   23-26
    24-25   25-26   25-32   26-27   27-31   33-34   34-35   35-36   36-37   37-38   38-39
    40-41   41-42   42-43   42-47   43-44   44-45   44-49   45-46   47-48   48-49

G1:H,SO3H

G2:O,S,[*1]

G3:[*2-*3],[*4-*5]

Match level :
    1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   6:Atom   7:Atom   8:Atom   9:Atom
    10:CLASS   11:CLASS   12:CLASS   14:CLASS   16:CLASS   18:Atom   19:Atom   20:Atom
    21:Atom   22:Atom   23:Atom   24:Atom   25:Atom   26:Atom   27:CLASS   28:CLASS
    29:CLASS   31:CLASS   32:CLASS   33:CLASS   34:CLASS   35:CLASS   36:CLASS
    37:CLASS   38:CLASS   39:CLASS   40:CLASS   41:CLASS   42:Atom   43:Atom   44:Atom
    45:CLASS   46:CLASS   47:Atom   48:Atom   49:Atom
Generic attributes :

14:
Type of chain   : Linear
Number of Carbon Atoms   : less than 7
27:
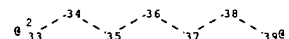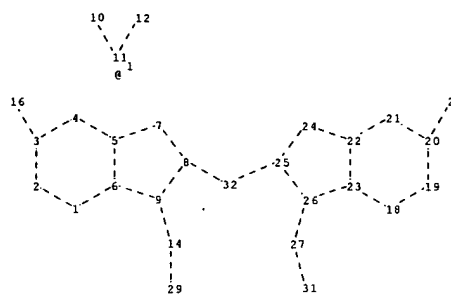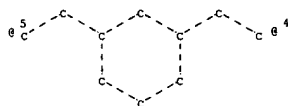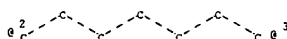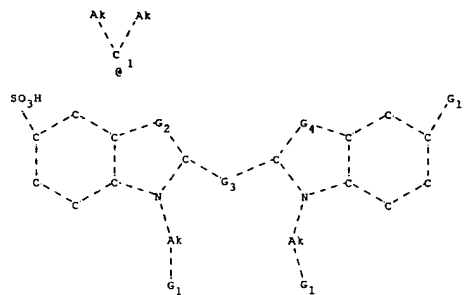Type of chain   : Linear
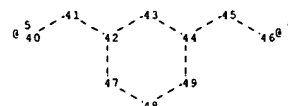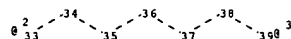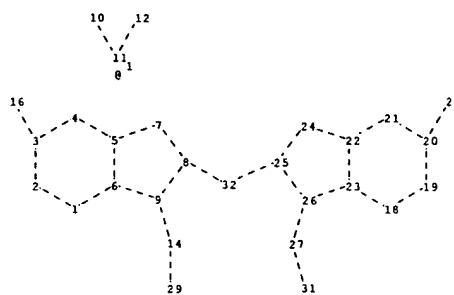Number of Carbon Atoms   : less than 7

chain nodes :
    10   11   12   14   16   27   28   29   31   32   33   34   35   36   37   38   39   40   41
    45   46
ring nodes :
    1   2   3   4   5   6   7   8   9   18   19   20   21   22   23   24   25   26   42   43   44
    47   48   49
chain bonds :
    3-16   8-32   9-14   10-11   11-12   14-29   20-28   25-32   26-27   27-31   33-34
    34-35   35-36   36-37   37-38   38-39   40-41   41-42   44-45   45-46
ring bonds :
    1-2   1-6   2-3   3-4   4-5   5-6   5-7   6-9   7-8   8-9   18-19   18-23   19-20
    20-21   21-22   22-23   22-24   23-26   24-25   25-26   42-43   42-47   43-44   44-49
    47-48   48-49
exact/norm bonds :
    1-2   1-6   2-3   3-4   3-16   4-5   5-6   5-7   6-9   7-8   8-9   8-32   9-14   10-11
    11-12   14-29   18-19   18-23   19-20   20-21   20-28   21-22   22-23   22-24   23-26
    24-25   25-26   25-32   26-27   27-31   33-34   34-35   35-36   36-37   37-38   38-39
    40-41   41-42   42-43   42-47   43-44   44-45   44-49   45-46   47-48   48-49

G1:H,SO3H

G2:O,S,[*1]

G3:[*2-*3],[*4-*5]

Match level :
    1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   6:Atom   7:Atom   8:Atom   9:Atom
    10:CLASS   11:CLASS   12:CLASS   14:CLASS   16:CLASS   18:Atom   19:Atom   20:Atom
    21:Atom   22:Atom   23:Atom   24:Atom   25:Atom   26:Atom   27:CLASS   28:CLASS
    29:CLASS   31:CLASS   32:CLASS   33:CLASS   34:CLASS   35:CLASS   36:CLASS
    37:CLASS   38:CLASS   39:CLASS   40:CLASS   41:CLASS   42:Atom   43:Atom   44:Atom
    45:CLASS   46:CLASS   47:Atom   48:Atom   49:Atom
Generic attributes :

```
10:
Type of chain              : Linear
Number of Carbon Atoms : less than 7
12:
Type of chain              : Linear
Number of Carbon Atoms : less than 7
14:
Type of chain              : Linear
Number of Carbon Atoms : less than 7
27:
Type of chain              : Linear
Number of Carbon Atoms : less than 7
```
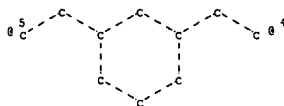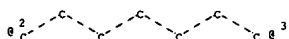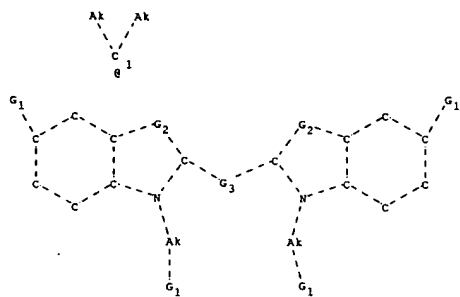
chain nodes :
    10   11   12   14   16   27   28   29   31   32   33   34   35   36   37   38   39   40   41
    45   46
ring nodes :
    1   2   3   4   5   6   7   8   9   18   19   20   21   22   23   24   25   26   42   43   44
    47   48   49
chain bonds :
    3-16   8-32   9-14   10-11   11-12   14-29   20-28   25-32   26-27   27-31   33-34
    34-35   35-36   36-37   37-38   38-39   40-41   41-42   44-45   45-46
ring bonds :
    1-2   1-6   2-3   3-4   4-5   5-6   5-7   6-9   7-8   8-9   18-19   18-23   19-20
    20-21   21-22   22-23   22-24   23-26   24-25   25-26   42-43   42-47   43-44   44-49
    47-48   48-49
exact/norm bonds :
    1-2   1-6   2-3   3-4   3-16   4-5   5-6   5-7   6-9   7-8   8-9   8-32   9-14   10-11
    11-12   14-29   18-19   18-23   19-20   20-21   20-28   21-22   22-23   22-24   23-26
    24-25   25-26   25-32   26-27   27-31   33-34   34-35   35-36   36-37   37-38   38-39
    40-41   41-42   42-43   42-47   43-44   44-45   44-49   45-46   47-48   48-49

G1:H,SO3H

G2:O,S,[*1]

G3:[*2-*3],[*4-*5]
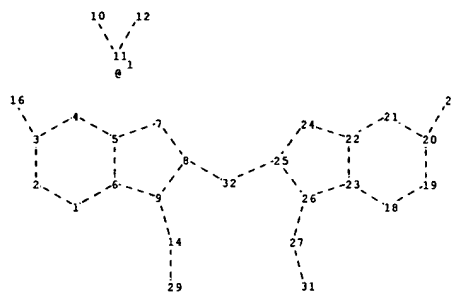
G4:S,[*1]
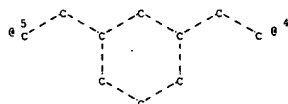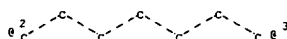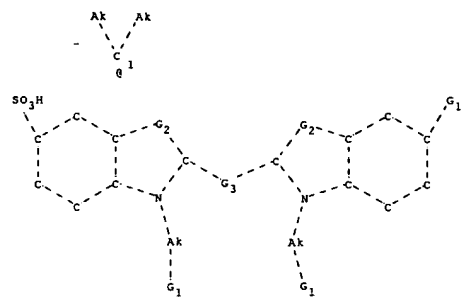
Match level :
    1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   6:Atom   7:Atom   8:Atom   9:Atom
    10:CLASS   11:CLASS   12:CLASS   14:CLASS   16:CLASS   18:Atom   19:Atom   20:Atom
    21:Atom   22:Atom   23:Atom   24:Atom   25:Atom   26:Atom   27:CLASS   28:CLASS
    29:CLASS   31:CLASS   32:CLASS   33:CLASS   34:CLASS   35:CLASS   36:CLASS
    37:CLASS   38:CLASS   39:CLASS   40:CLASS   41:CLASS   42:Atom   43:Atom   44:Atom
    45:CLASS

```
                46:CLASS    47:Atom    48:Atom    49:Atom
Generic attributes :
     10:
     Type of chain            : Linear
     Number of Carbon Atoms : less than 7
     12:
     Type of chain            : Linear
     Number of Carbon Atoms : less than 7
     14:
     Type of chain            : Linear
     Number of Carbon Atoms : less than 7
     27:
     Type of chain            : Linear
     Number of Carbon Atoms : less than 7
```

chain nodes :
     10   11   12   14   16   27   28   29   31   32   33   34   35   36   37   38   39   40   41
     45   46
ring nodes :
     1   2   3   4   5   6   7   8   9   18   19   20   21   22   23   24   25   26   42   43   44
     47   48   49
chain bonds :
     3-16   8-32   9-14   10-11   11-12   14-29   20-28   25-32   26-27   27-31   33-34
     34-35   35-36   36-37   37-38   38-39   40-41   41-42   44-45   45-46
ring bonds :
     1-2   1-6   2-3   3-4   4-5   5-6   5-7   6-9   7-8   8-9   18-19   18-23   19-20
     20-21   21-22   22-23   22-24   23-26   24-25   25-26   42-43   42-47   43-44   44-49
     47-48   48-49
exact/norm bonds :
     1-2   1-6   2-3   3-4   3-16   4-5   5-6   5-7   6-9   7-8   8-9   8-32   9-14   10-11
     11-12   14-29   18-19   18-23   19-20   20-21   20-28   21-22   22-23   22-24   23-26
     24-25   25-26   25-32   26-27   27-31   33-34   34-35   35-36   36-37   37-38   38-39
     40-41   41-42   42-43   42-47   43-44   44-45   44-49   45-46   47-48   48-49

G1:H,SO3H

G2:O,S,[*1]

G3:[*2-*3],[*4-*5]

G4:S,[*1]
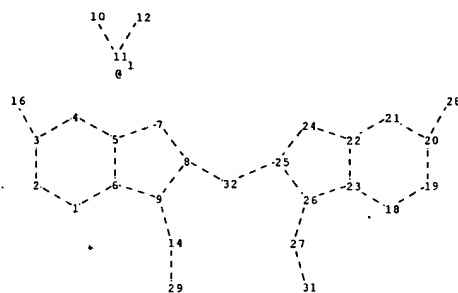
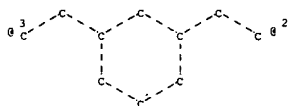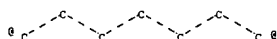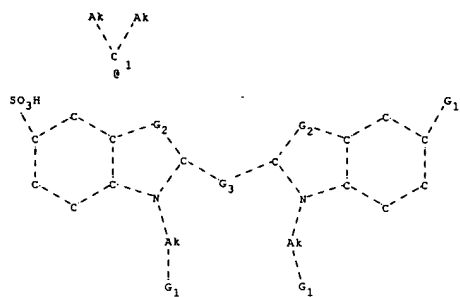Match level :
     1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   6:Atom   7:Atom   8:Atom   9:Atom
     10:CLASS   11:CLASS   12:CLASS   14:CLASS   16:CLASS   18:Atom   19:Atom   20:Atom
     21:Atom   22:Atom   23:Atom   24:Atom   25:Atom   26:Atom   27:CLASS   28:CLASS
     29:CLASS   31:CLASS   32:CLASS   33:CLASS   34:CLASS   35:CLASS   36:CLASS
     37:CLASS   38:CLASS   39:CLASS   40:CLASS   41:CLASS   42:Atom   43:Atom   44:Atom
     45:CLASS

```
          46:CLASS   47:Atom   48:Atom   49:Atom
Generic attributes :
     10:
     Type of chain          : Linear
     Number of Carbon Atoms : less than 7
     12:
     Type of chain          : Linear
     Number of Carbon Atoms : less than 7
     14:
     Type of chain          : Linear
     Number of Carbon Atoms : less than 7
     27:
     Type of chain          : Linear
     Number of Carbon Atoms : less than 7
```

chain nodes :
    10   11   12   14   16   27   28   29   31   32   33   34   35   36   37   38   39   40   41
    45   46
ring nodes :
    1   2   3   4   5   6   7   8   9   18   19   20   21   22   23   24   25   26   42   43   44
    47   48   49
chain bonds :
    3-16   8-32   9-14   10-11   11-12   14-29   20-28   25-32   26-27   27-31   33-34
    34-35   35-36   36-37   37-38   38-39   40-41   41-42   44-45   45-46
ring bonds :
    1-2   1-6   2-3   3-4   4-5   5-6   5-7   6-9   7-8   8-9   18-19   18-23   19-20
    20-21   21-22   22-23   22-24   23-26   24-25   25-26   42-43   42-47   43-44   44-49
    47-48   48-49
exact/norm bonds :
    1-2   1-6   2-3   3-4   3-16   4-5   5-6   5-7   6-9   7-8   8-9   8-32   9-14   10-11
    11-12   14-29   18-19   18-23   19-20   20-21   20-28   21-22   22-23   22-24   23-26
    24-25   25-26   25-32   26-27   27-31   33-34   34-35   35-36   36-37   37-38   38-39
    40-41   41-42   42-43   42-47   43-44   44-45   44-49   45-46   47-48   48-49

G1:H,SO3H

G2:O,S,[*1]

G3:[*2-*3],[*4-*5]

G4:S,[*1]

Hydrogen count :
    36:= exact 0   43:= exact 0
Connectivity :
    36:3 E exact RC ring/chain   43:3 E exact RC ring/chain
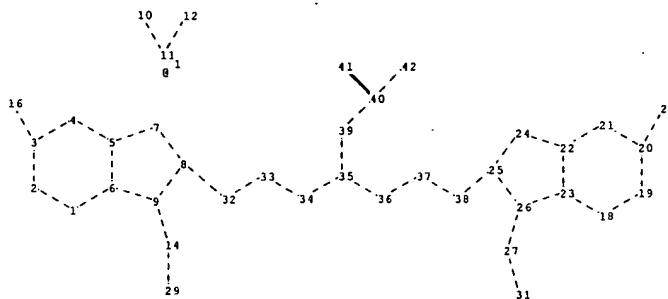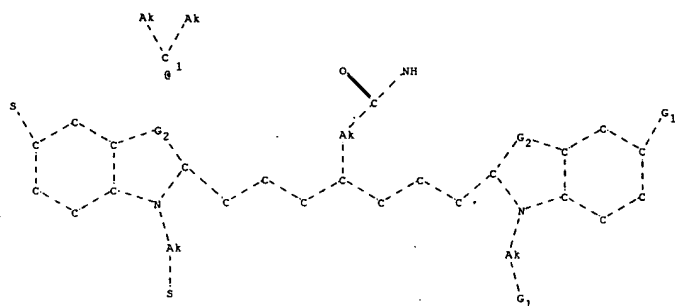Match level :
    1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   6:Atom   7:Atom   8:Atom   9:Atom
    10:CLASS

```
           11:CLASS   12:CLASS   14:CLASS   16:CLASS   18:Atom   19:Atom   20:Atom
      21:Atom   22:Atom   23:Atom   24:Atom   25:Atom   26:Atom   27:CLASS   28:CLASS
      29:CLASS   31:CLASS   32:CLASS   33:CLASS   34:CLASS   35:CLASS   36:CLASS
      37:CLASS   38:CLASS   39:CLASS   40:CLASS   41:CLASS   42:Atom   43:Atom   44:Atom
      45:CLASS   46:CLASS   47:Atom   48:Atom   49:Atom
Generic attributes :
      10:
      Type of chain            : Linear
      Number of Carbon Atoms : less than 7
      12:
      Type of chain            : Linear
      Number of Carbon Atoms : less than 7
      14:
      Type of chain            : Linear
      Number of Carbon Atoms : less than 7
      27:
      Type of chain            : Linear
      Number of Carbon Atoms : less than 7
```

chain nodes :
    10   11   12   14   16   27   28   29   31   32   33   34   35   36   37   38   39   40   41
    45   46
ring nodes :
    1   2   3   4   5   6   7   8   9   18   19   20   21   22   23   24   25   26   42   43   44
    47   48   49
chain bonds :
    3-16   8-32   9-14   10-11   11-12   14-29   20-28   25-32   26-27   27-31   33-34
    34-35   35-36   36-37   37-38   38-39   40-41   41-42   44-45   45-46
ring bonds :
    1-2   1-6   2-3   3-4   4-5   5-6   5-7   6-9   7-8   8-9   18-19   18-23   19-20
    20-21   21-22   22-23   22-24   23-26   24-25   25-26   42-43   42-47   43-44   44-49
    47-48   48-49
exact/norm bonds :
    1-2   1-6   2-3   3-4   3-16   4-5   5-6   5-7   6-9   7-8   8-9   8-32   9-14   10-11
    11-12   14-29   18-19   18-23   19-20   20-21   20-28   21-22   22-23   22-24   23-26
    24-25   25-26   25-32   26-27   27-31   33-34   34-35   35-36   36-37   37-38   38-39
    40-41   41-42   42-43   42-47   43-44   44-45   44-49   45-46   47-48   48-49

G1:H,SO3H

G2:O,S,[*1]

G3:[*2-*3],[*4-*5]

G4:S,[*1]

Hydrogen count :
    36:= exact 0   43:= exact 0
Connectivity :
    36:3 E exact RC ring/chain   43:3 E exact RC ring/chain
Match level :
    1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   6:Atom   7:Atom   8:Atom   9:Atom
    10:CLASS

```
          11:CLASS   12:CLASS   14:CLASS    16:CLASS    18:Atom    19:Atom    20:Atom
   21:Atom   22:Atom   23:Atom    24:Atom    25:Atom    26:Atom    27:CLASS    28:CLASS
   29:CLASS   31:CLASS   32:CLASS    33:CLASS  34:CLASS    35:CLASS    36:CLASS
   37:CLASS   38:CLASS   39:CLASS    40:CLASS    41:CLASS    42:Atom    43:Atom    44:Atom
   45:CLASS   46:CLASS   47:Atom    48:Atom    49:Atom
```
Generic attributes :
```
   10:
   Type of chain            : Linear
   Number of Carbon Atoms : less than 7
   12:
   Type of chain            : Linear
   Number of Carbon Atoms : less than 7
   14:
   Type of chain            : Linear
   Number of Carbon Atoms : less than 7
   27:
   Type of chain            : Linear
   Number of Carbon Atoms : less than 7
```

chain nodes :
     10   11   12   14   16   27   28   29   31   32   33   34   35   36   37   38   39   40   41
     45   46
ring nodes :
     1   2   3   4   5   6   7   8   9   18   19   20   21   22   23   24   25   26   42   43   44
     47   48   49
chain bonds :
     3-16   8-32   9-14   10-11   11-12   14-29   20-28   25-32   26-27   27-31   33-34
     34-35   35-36   36-37   37-38   38-39   40-41   41-42   44-45   45-46
ring bonds :
     1-2   1-6   2-3   3-4   4-5   5-6   5-7   6-9   7-8   8-9   18-19   18-23   19-20
     20-21   21-22   22-23   22-24   23-26   24-25   25-26   42-43   42-47   43-44   44-49
     47-48   48-49
exact/norm bonds :
     1-2   1-6   2-3   3-4   3-16   4-5   5-6   5-7   6-9   7-8   8-9   8-32   9-14   10-11
     11-12   14-29   18-19   18-23   19-20   20-21   20-28   21-22   22-23   22-24   23-26
     24-25   25-26   25-32   26-27   27-31   33-34   34-35   35-36   36-37   37-38   38-39
     40-41   41-42   42-43   42-47   43-44   44-45   44-49   45-46   47-48   48-49

G1:H,SO3H

G2:O,S,[*1]

G3:[*2-*3]

G4:S,[*1]

Hydrogen count :
     36:= exact 0   43:= exact 0
Connectivity :
     36:3 E exact RC ring/chain   43:3 E exact RC ring/chain
Match level :
   1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   6:Atom   7:Atom   8:Atom   9:Atom
     10:CLASS

```
            11:CLASS    12:CLASS    14:CLASS    16:CLASS    18:Atom    19:Atom    20:Atom
    21:Atom    22:Atom    23:Atom    24:Atom    25:Atom    26:Atom    27:CLASS    28:CLASS
    29:CLASS    31:CLASS    32:CLASS    33:CLASS    34:CLASS    35:CLASS    36:CLASS
    37:CLASS    38:CLASS    39:CLASS    40:CLASS    41:CLASS    42:Atom    43:Atom    44:Atom
    45:CLASS    46:CLASS    47:Atom    48:Atom    49:Atom
Generic attributes :
    10:
    Type of chain              : Linear
    Number of Carbon Atoms : less than 7
    12:
    Type of chain              : Linear
    Number of Carbon Atoms : less than 7
    14:
    Type of chain              : Linear
    Number of Carbon Atoms : less than 7
    27:
    Type of chain              : Linear
    Number of Carbon Atoms : less than 7
```

chain nodes :
    10   11   12   14   16   27   28   29   31   32   33   37   38   39   40   41   42
ring nodes :
    1   2   3   4   5   6   7   8   9   18   19   20   21   22   23   24   25   26
ring/chain nodes :
    34   35   36
chain bonds :
    3-16   8-32   9-14   10-11   11-12   14-29   20-28   25-38   26-27   27-31   32-33
    33-34   35-39   36-37   37-38   39-40   40-41   40-42
ring/chain bonds :
    34-35   35-36
ring bonds :
    1-2   1-6   2-3   3-4   4-5   5-6   5-7   6-9   7-8   8-9   18-19   18-23   19-20
    20-21   21-22   22-23   22-24   23-26   24-25   25-26
exact/norm bonds :
    1-2   1-6   2-3   3-4   3-16   4-5   5-6   5-7   6-9   7-8   8-9   8-32   9-14   10-11
    11-12   14-29   18-19   18-23   19-20   20-21   20-28   21-22   22-23   22-24   23-26
    24-25   25-26   25-38   26-27   27-31   32-33   33-34   34-35   35-36   35-39   36-37
    37-38   39-40   40-41   40-42


G1:H,SO3H

G2:O,S,[*1]

Match level :
    1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   6:Atom   7:Atom   8:Atom   9:Atom
    10:CLASS   11:CLASS   12:CLASS   14:CLASS   16:CLASS   18:Atom   19:Atom   20:Atom
    21:Atom   22:Atom   23:Atom   24:Atom   25:Atom   26:Atom   27:CLASS   28:CLASS
    29:CLASS   31:CLASS   32:CLASS   33:CLASS   34:CLASS   35:CLASS   36:CLASS
    37:CLASS   38:CLASS   39:CLASS   40:CLASS   41:CLASS   42:CLASS
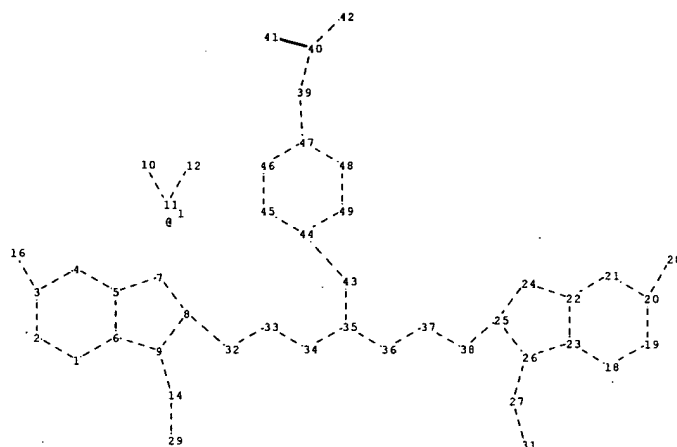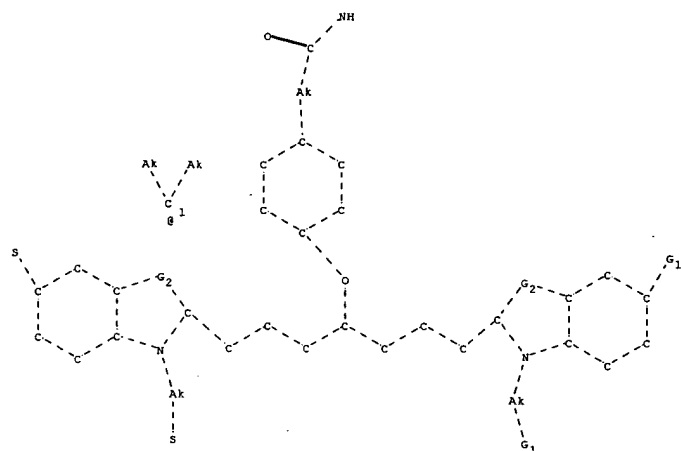
chain nodes :
    10   11   12   14   16   27   28   29   31   32   33   37   38   39   40   41   42   43
ring nodes :
    1   2   3   4   5   6   7   8   9   18   19   20   21   22   23   24   25   26   44   45   46
    47   48   49
ring/chain nodes :
    34   35   36
chain bonds :
    3-16   8-32   9-14   10-11   11-12   14-29   20-28   25-38   26-27   27-31   32-33
    33-34   35-43   36-37   37-38   39-40   39-47   40-41   40-42   43-44
ring/chain bonds :
    34-35   35-36
ring bonds :
    1-2   1-6   2-3   3-4   4-5   5-6   5-7   6-9   7-8   8-9   18-19   18-23   19-20
    20-21   21-22   22-23   22-24   23-26   24-25   25-26   44-45   44-49   45-46   46-47
    47-48   48-49
exact/norm bonds :
    1-2   1-6   2-3   3-4   3-16   4-5   5-6   5-7   6-9   7-8   8-9   8-32   9-14   10-11
    11-12   14-29   18-19   18-23   19-20   20-21   20-28   21-22   22-23   22-24   23-26
    24-25   25-26   25-38   26-27   27-31   32-33   33-34   34-35   35-36   35-43   36-37
    37-38   39-40   39-47   40-41   40-42   43-44   44-45   44-49   45-46   46-47   47-48
    48-49


G1:H,SO3H

G2:O,S,[*1]

Match level :
    1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   6:Atom   7:Atom   8:Atom   9:Atom
    10:CLASS   11:CLASS   12:CLASS   14:CLASS   16:CLASS   18:Atom   19:Atom   20:Atom
    21:Atom   22:Atom   23:Atom   24:Atom   25:Atom   26:Atom   27:CLASS   28:CLASS
    29:CLASS   31:CLASS   32:CLASS   33:CLASS   34:CLASS   35:CLASS   36:CLASS
    37:CLASS   38:CLASS   39:CLASS   40:CLASS   41:CLASS   42:CLASS   43:CLASS
    44:Atom

```
          45:Atom    46:Atom    47:Atom    48:Atom    49:Atom
Generic attributes :
    39:
    Type of chain          : Linear
    Number of Carbon Atoms : less than 7
```
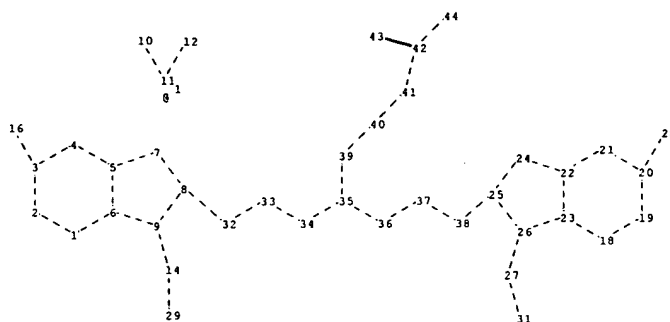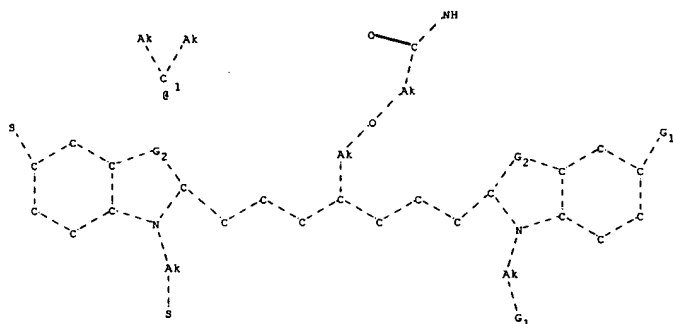
```
chain nodes :
    10   11   12   14   16   27   28   29   31   32   33   37   38   39   40   41   42   43   44
ring nodes :
    1    2    3    4    5    6    7    8    9    18   19   20   21   22   23   24   25   26
ring/chain nodes :
    34   35   36
chain bonds :
    3-16   8-32   9-14   10-11   11-12   14-29   20-28   25-38   26-27   27-31   32-33
    33-34   35-39   36-37   37-38   39-40   40-41   41-42   42-43   42-44
ring/chain bonds :
    34-35   35-36
ring bonds :
    1-2    1-6    2-3    3-4    4-5    5-6    5-7    6-9    7-8    8-9    18-19   18-23   19-20
    20-21   21-22   22-23   22-24   23-26   24-25   25-26
exact/norm bonds :
    1-2    1-6    2-3    3-4    3-16   4-5    5-6    5-7    6-9    7-8    8-9    8-32   9-14   10-11
    11-12   14-29   18-19   18-23   19-20   20-21   20-28   21-22   22-23   22-24   23-26
    24-25   25-26   25-38   26-27   27-31   32-33   33-34   34-35   35-36   35-39   36-37
    37-38   39-40   40-41   41-42   42-43   42-44
```

G1:H,SO3H

G2:O,S,[*1]

```
Match level :
    1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   6:Atom   7:Atom   8:Atom   9:Atom
    10:CLASS   11:CLASS   12:CLASS   14:CLASS   16:CLASS   18:Atom   19:Atom   20:Atom
    21:Atom   22:Atom   23:Atom   24:Atom   25:Atom   26:Atom   27:CLASS   28:CLASS
    29:CLASS   31:CLASS   32:CLASS   33:CLASS   34:CLASS   35:CLASS   36:CLASS
    37:CLASS   38:CLASS   39:CLASS   40:CLASS   41:CLASS   42:CLASS   43:CLASS
    44:CLASS
Generic attributes :
    41:
```

```
Type of chain           : Linear
Number of Carbon Atoms  : less than 7
```
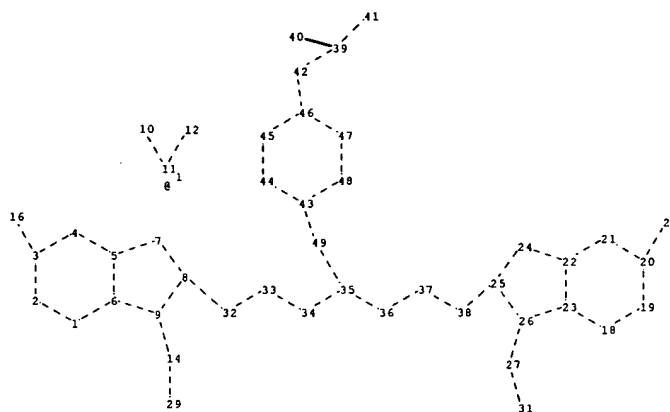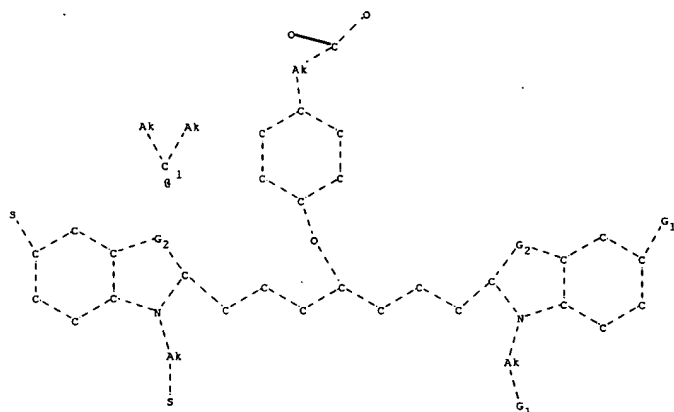
```
chain nodes :
    10   11   12   14   16   27   28   29   31   32   33   37   38   39   40   41   42   49
ring nodes :
    1    2    3    4    5    6    7    8    9    18   19   20   21   22   23   24   25   26   43   44   45
    46   47   48
ring/chain nodes :
    34   35   36
chain bonds :
    3-16   8-32   9-14   10-11   11-12   14-29   20-28   25-38   26-27   27-31   32-33
    33-34   35-49   36-37   37-38   39-41   39-40   39-42   42-46   43-49
ring/chain bonds :
    34-35   35-36
ring bonds :
    1-2    1-6    2-3    3-4    4-5    5-6    5-7    6-9    7-8    8-9    18-19   18-23   19-20
    20-21   21-22   22-23   22-24   23-26   24-25   25-26   43-44   43-48   44-45   45-46
    46-47   47-48
exact/norm bonds :
    1-2    1-6    2-3    3-4    3-16   4-5    5-6    5-7    6-9    7-8    8-9    8-32   9-14   10-11
    11-12   14-29   18-19   18-23   19-20   20-21   20-28   21-22   22-23   22-24   23-26
    24-25   25-26   25-38   26-27   27-31   32-33   33-34   34-35   35-36   35-49   36-37
    37-38   39-41   39-40   39-42   42-46   43-44   43-48   43-49   44-45   45-46   46-47
    47-48


G1:H,SO3H

G2:O,S,[*1]

Match level :
    1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   6:Atom   7:Atom   8:Atom   9:Atom
    10:CLASS   11:CLASS   12:CLASS   14:CLASS   16:CLASS   18:Atom   19:Atom   20:Atom
    21:Atom   22:Atom   23:Atom   24:Atom   25:Atom   26:Atom   27:CLASS   28:CLASS
    29:CLASS   31:CLASS   32:CLASS   33:CLASS   34:CLASS   35:CLASS   36:CLASS
    37:CLASS   38:CLASS   39:CLASS   40:CLASS   41:CLASS   42:CLASS   43:CLASS
    44:CLASS
```

45:Atom   46:Atom   47:Atom   48:Atom   49:CLASS
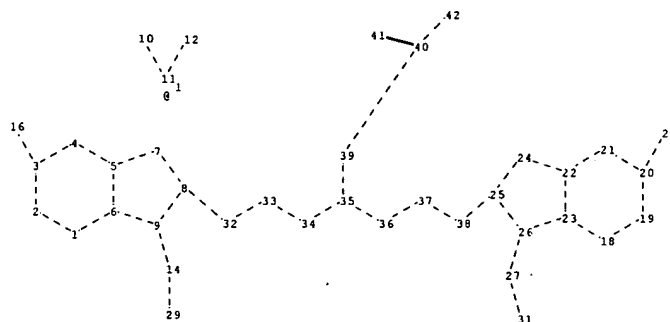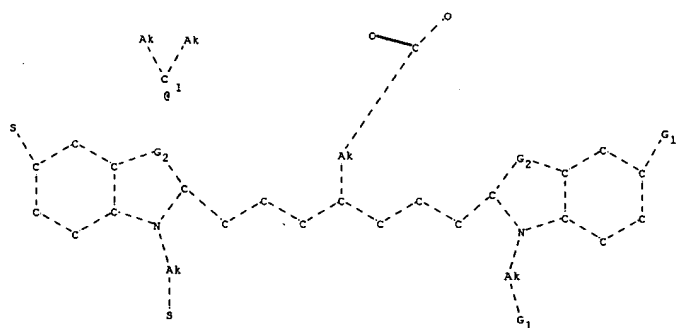
45:Atom   46:Atom   47:Atom   48:Atom   49:CLASS

chain nodes :
    10   11   12   14   16   27   28   29   31   32   33   37   38   39   40   41   42
ring nodes :
    1   2   3   4   5   6   7   8   9   18   19   20   21   22   23   24   25   26
ring/chain nodes :
    34   35   36
chain bonds :
    3-16   8-32   9-14   10-11   11-12   14-29   20-28   25-38   26-27   27-31   32-33
    33-34   35-39   36-37   37-38   39-40   40-42   40-41
ring/chain bonds :
    34-35   35-36
ring bonds :
    1-2   1-6   2-3   3-4   4-5   5-6   5-7   6-9   7-8   8-9   18-19   18-23   19-20
    20-21   21-22   22-23   22-24   23-26   24-25   25-26
exact/norm bonds :
    1-2   1-6   2-3   3-4   3-16   4-5   5-6   5-7   6-9   7-8   8-9   8-32   9-14   10-11
    11-12   14-29   18-19   18-23   19-20   20-21   20-28   21-22   22-23   22-24   23-26
    24-25   25-26   25-38   26-27   27-31   32-33   33-34   34-35   35-36   35-39   36-37
    37-38   39-40   40-42   40-41

G1:H,SO3H

G2:O,S,[*1]

Match level :
    1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   6:Atom   7:Atom   8:Atom   9:Atom
    10:CLASS   11:CLASS   12:CLASS   14:CLASS   16:CLASS   18:Atom   19:Atom   20:Atom
    21:Atom   22:Atom   23:Atom   24:Atom   25:Atom   26:Atom   27:CLASS   28:CLASS
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    37:CLASS   38:CLASS   39:CLASS   40:CLASS   41:CLASS   42:CLASS
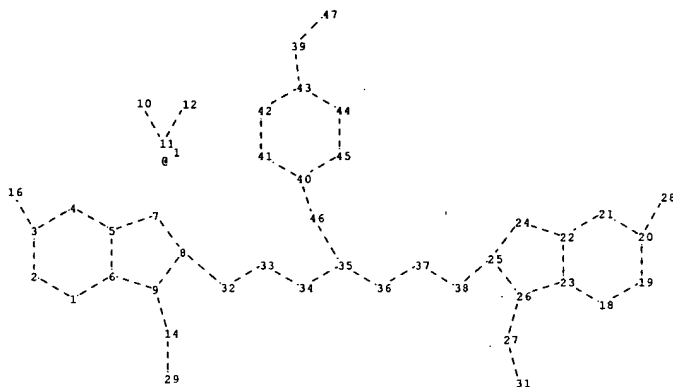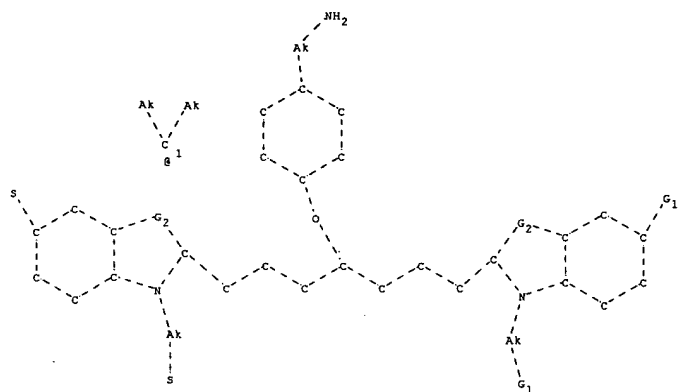
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chain nodes :
    10   11   12   14   16   27   28   29   31   32   33   37   38   39   46   47
ring nodes :
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    43   44   45
ring/chain nodes :
    34   35   36
chain bonds :
    3-16   8-32   9-14   10-11   11-12   14-29   20-28   25-38   26-27   27-31   32-33
    33-34   35-46   36-37   37-38   39-43   39-47   40-46
ring/chain bonds :
    34-35   35-36
ring bonds :
    1-2    1-6    2-3    3-4    4-5    5-6    5-7    6-9    7-8    8-9    18-19   18-23   19-20
    20-21  21-22  22-23  22-24  23-26  24-25  25-26  40-41   40-45   41-42   42-43
    43-44  44-45
exact/norm bonds :
    1-2    1-6    2-3    3-4    3-16   4-5    5-6    5-7    6-9    7-8    8-9    8-32   9-14   10-11
    11-12  14-29  18-19  18-23  19-20  20-21  20-28  21-22  22-23  22-24  23-26
    24-25  25-26  25-38  26-27  27-31  32-33  33-34  34-35  35-36  35-46  36-37
    37-38  39-43  39-47  40-41  40-45  40-46  41-42  42-43  43-44  44-45


G1:H,SO3H

G2:O,S,[*1]

Match level :
    1:Atom    2:Atom    3:Atom    4:Atom    5:Atom    6:Atom    7:Atom    8:Atom    9:Atom
    10:CLASS   11:CLASS   12:CLASS   14:CLASS   16:CLASS   18:Atom   19:Atom   20:Atom
    21:Atom   22:Atom   23:Atom   24:Atom   25:Atom   26:Atom   27:CLASS   28:CLASS
    29:CLASS   31:CLASS   32:CLASS   33:CLASS   34:CLASS   35:CLASS   36:CLASS
    37:CLASS   38:CLASS   39:CLASS   40:CLASS   41:CLASS   42:Atom   43:Atom   44:Atom
    45:Atom   46:CLASS   47:CLASS
```
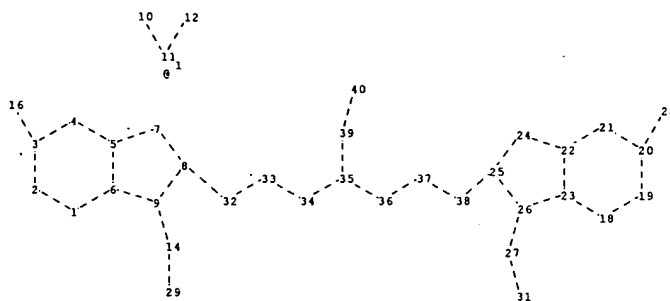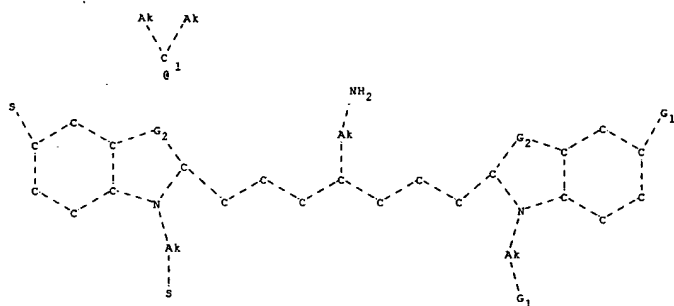
chain nodes :
    10   11   12   14   16   27   28   29   31   32   33   37   38   39   40
ring nodes :
    1   2   3   4   5   6   7   8   9   18   19   20   21   22   23   24   25   26
ring/chain nodes :
    34   35   36
chain bonds :
    3-16   8-32   9-14   10-11   11-12   14-29   20-28   25-38   26-27   27-31   32-33
    33-34   35-39   36-37   37-38   39-40
ring/chain bonds :
    34-35   35-36
ring bonds :
    1-2   1-6   2-3   3-4   4-5   5-6   5-7   6-9   7-8   8-9   18-19   18-23   19-20
    20-21   21-22   22-23   22-24   23-26   24-25   25-26
exact/norm bonds :
    1-2   1-6   2-3   3-4   3-16   4-5   5-6   5-7   6-9   7-8   8-9   8-32   9-14   10-11
    11-12   14-29   18-19   18-23   19-20   20-21   20-28   21-22   22-23   22-24   23-26
    24-25   25-26   25-38   26-27   27-31   32-33   33-34   34-35   35-36   35-39   36-37
    37-38   39-40

G1:H,SO3H

G2:O,S,[*1]

Match level :
    1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   6:Atom   7:Atom   8:Atom   9:Atom
    10:CLASS   11:CLASS   12:CLASS   14:CLASS   16:CLASS   18:Atom   19:Atom   20:Atom
    21:Atom   22:Atom   23:Atom   24:Atom   25:Atom   26:Atom   27:CLASS   28:CLASS
    29:CLASS   31:CLASS   32:CLASS   33:CLASS   34:CLASS   35:CLASS   36:CLASS
    37:CLASS   38:CLASS   39:CLASS   40:CLASS

ACCESSION NUMBER: 2004:633995 HCAPLUS
DOCUMENT NUMBER: 141:158512
TITLE: Hydrophilic, thiol-reactive cyanine dyes and
                           conjugates thereof with biomolecules for fluorescence
   diagnosis
INVENTOR(S):   Licha, Kai; Perlitz, Christin
PATENT ASSIGNEE(S):   Schering Ag, Germany
SOURCE: PCT Int. Appl., 65 pp.
                           CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

        PATENT NO.   KIND   DATE   APPLICATION NO.   DATE
        --------------   ----   --------   --------------------   --------
        WO 2004065491   A1   20040805   WO 2003-EP12735   20031114 <--
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                CO, CR, CU, CZ, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM,
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                LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG,
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            RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,
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PRIORITY APPLN. INFO.:   DE 2003-10302787   A 20030124 <--
                                                 US 2003-443197P   P 20030129

OTHER SOURCE(S):   MARPAT 141:158512
IT   **731862-91-2P 731862-98-9P 731863-01-7P**
      731863-04-0P 731863-05-1P 731863-06-2P
      731863-08-4P 731863-09-5P 731863-10-8P
      RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT
      (Reactant or reagent)
         (manufacture of hydrophilic, thiol-reactive cyanine dyes and conjugates
         thereof with biomols. for fluorescence diagnosis)
RN   731862-91-2 HCAPLUS
CN   3H-Indolium, 2-[4-(2-carboxyethyl)-7-[1,3-dihydro-3,3-dimethyl-5-sulfo-1-
      (2-sulfoethyl)-2H-indol-2-ylidene]-1,3,5-heptatrienyl]-3,3-dimethyl-5-
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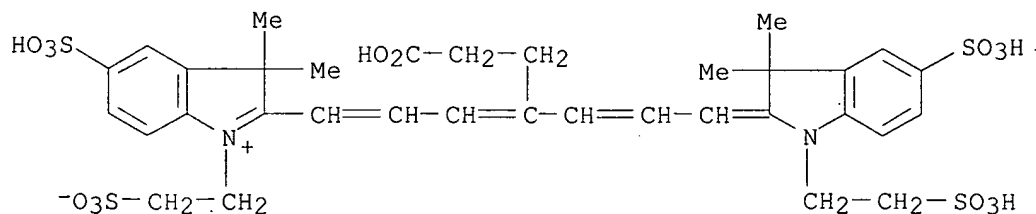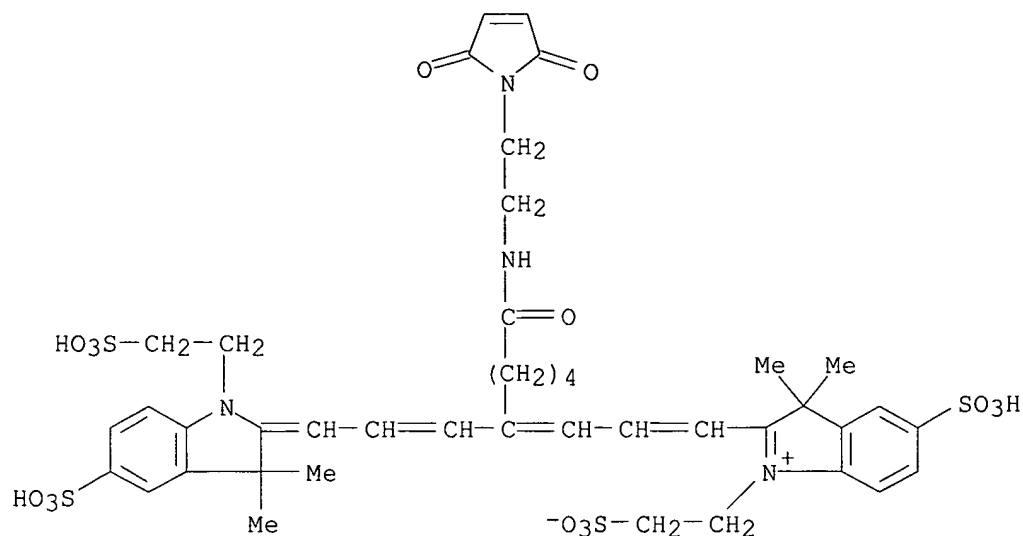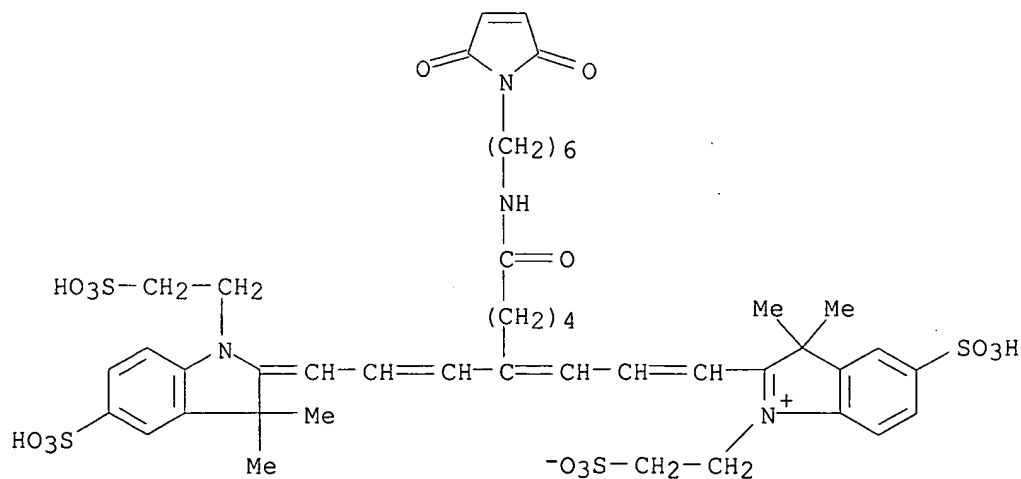

● 3 Na

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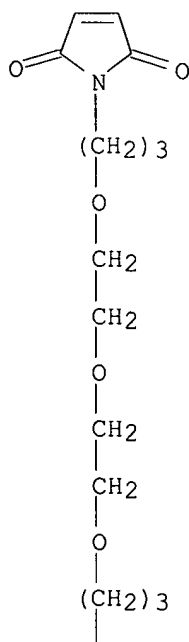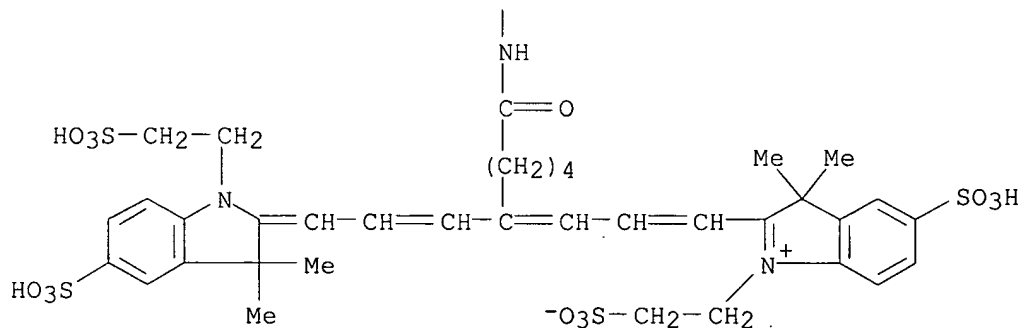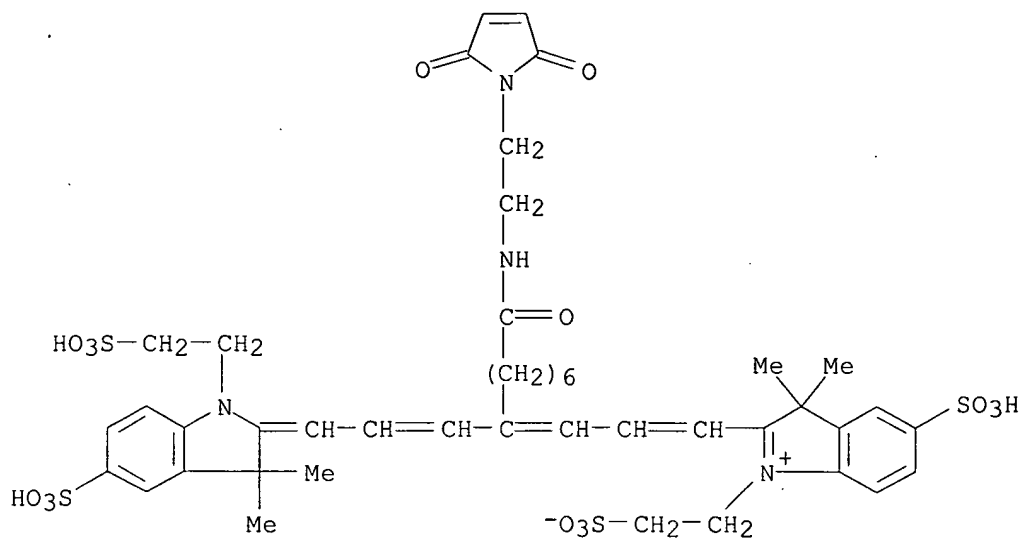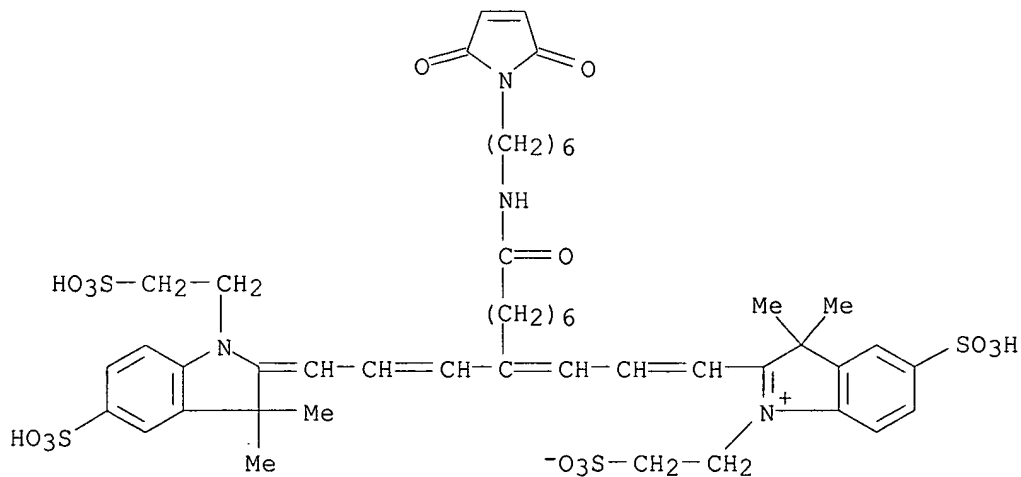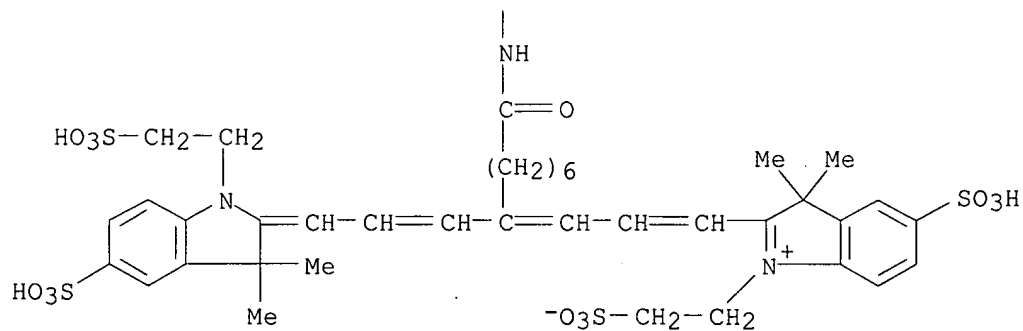CN   3H-Indolium, 2-[8-carboxy-4-[3-[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-
      sulfoethyl)-2H-indol-2-ylidene]-1-propenyl]-1,3-octadienyl]-3,3-dimethyl-5-
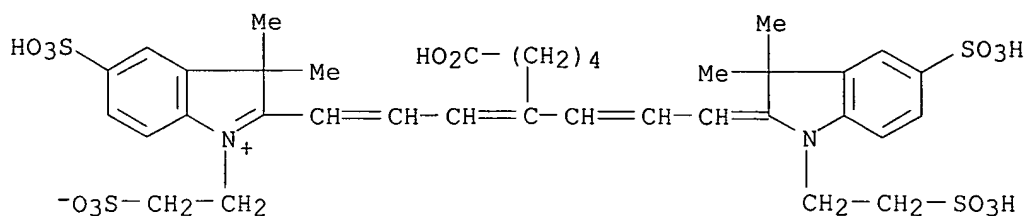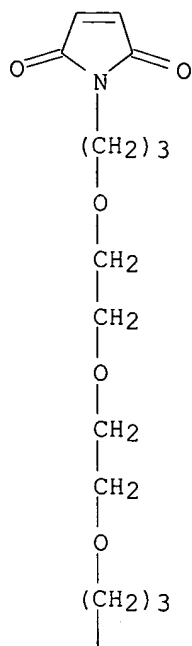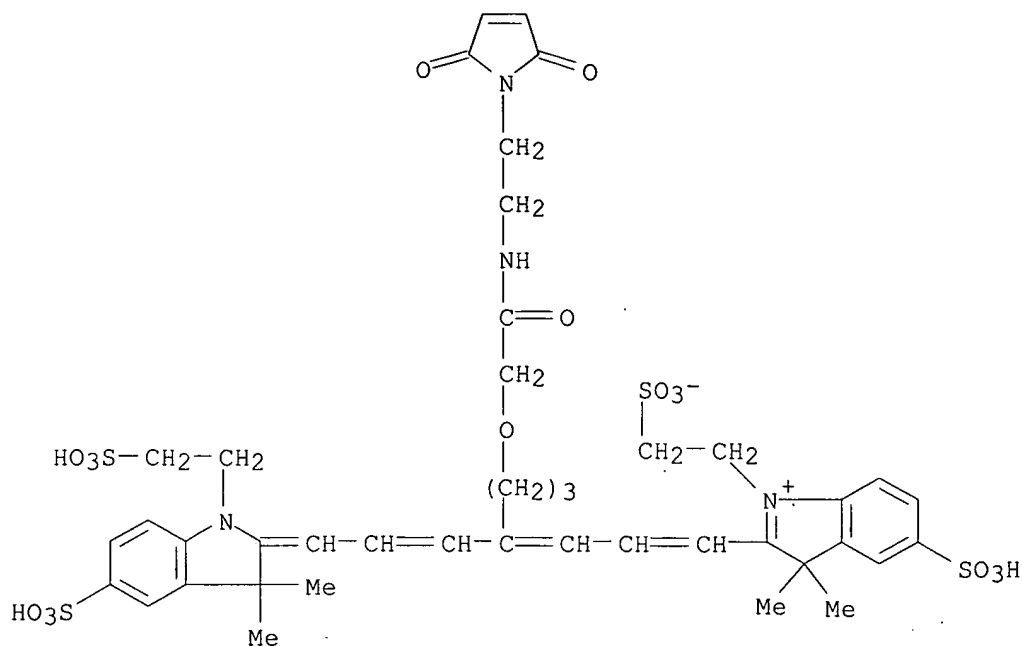
●3 Na

RN   731863-01-7   HCAPLUS
CN   3H-Indolium, 2-[10-carboxy-4-[3-[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-
      sulfoethyl)-2H-indol-2-ylidene]-1-propenyl]-1,3-decadienyl]-3,3-dimethyl-5-
      sulfo-1-(2-sulfoethyl)-, inner salt, trisodium salt (9CI)   (CA INDEX NAME)
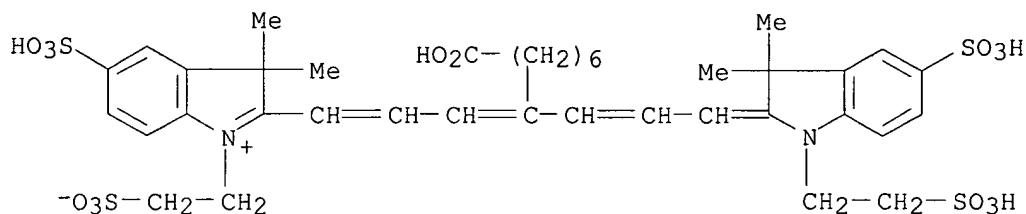
●3   Na

RN   731863-04-0   HCAPLUS
CN   3H-Indolium, 2-[4-[3-(2-carboxyethoxy)propyl]-7-[1,3-dihydro-3,3-dimethyl-
      5-sulfo-1-(2-sulfoethyl)-2H-indol-2-ylidene]-1,3,5-heptatrienyl]-3,3-
      dimethyl-5-sulfo-1-(2-sulfoethyl)-, inner salt, trisodium salt (9CI)   (CA
      INDEX NAME)
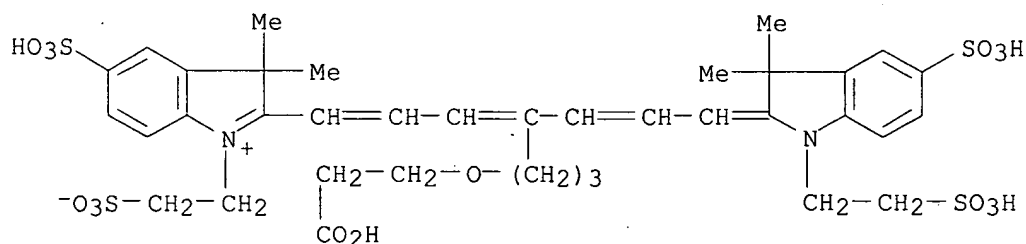
●3   Na

RN   731863-05-1   HCAPLUS
CN   3H-Indolium, 2-[2-[2-chloro-3-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-
      sulfoethyl)-2H-indol-2-ylidene]ethylidene]-1-cyclohexen-1-yl]ethenyl]-3,3-
      dimethyl-5-sulfo-1-(2-sulfoethyl)-, inner salt, trisodium salt (9CI)   (CA
      INDEX NAME)
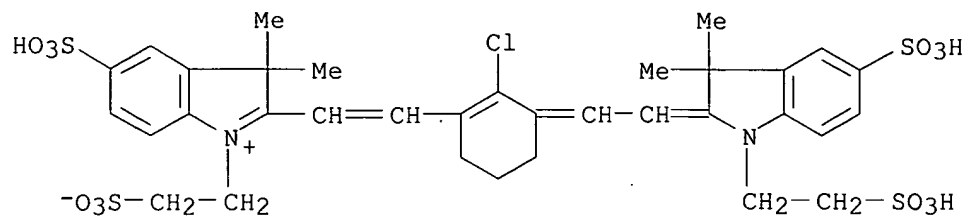
●3 Na

RN   731863-06-2   HCAPLUS
CN   3H-Indolium, 2-[2-[2-[4-(2-carboxyethyl)phenoxy]-3-[[1,3-dihydro-3,3-
     dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-indol-2-ylidene]ethylidene]-1-
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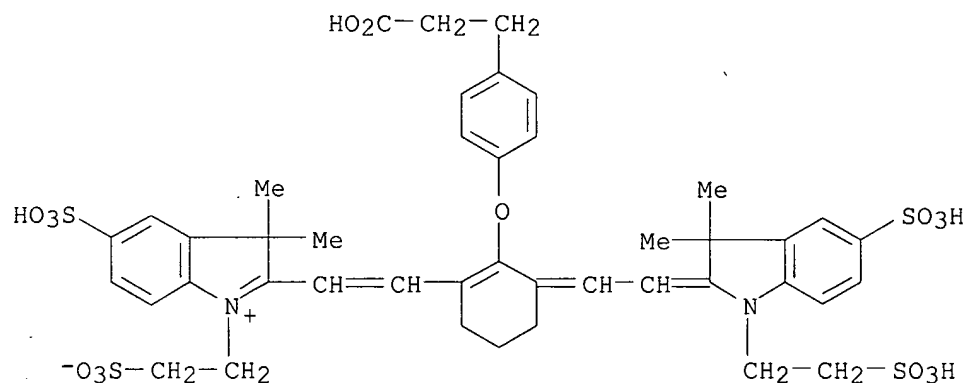
●3 Na

RN   731863-08-4   HCAPLUS
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     sulfoethyl)-2H-indol-2-ylidene]ethylidene]-5-(1,1-dimethylethyl)-1-
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     salt, trisodium salt (9CI)   (CA INDEX NAME)
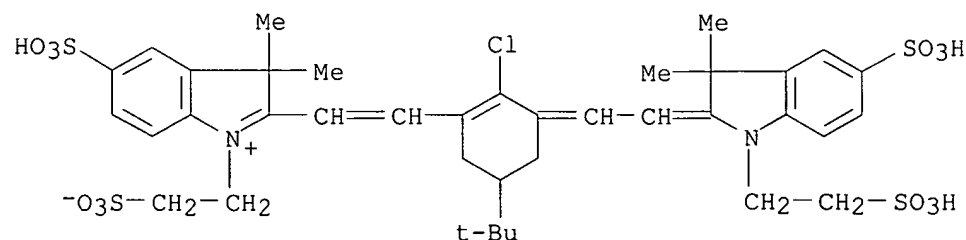
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RN 731863-09-5 HCAPLUS
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    dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-indol-2-ylidene]ethylidene]-5-(1,1-
    dimethylethyl)-1-cyclohexen-1-yl]ethenyl]-3,3-dimethyl-5-sulfo-1-(2-
    sulfoethyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)
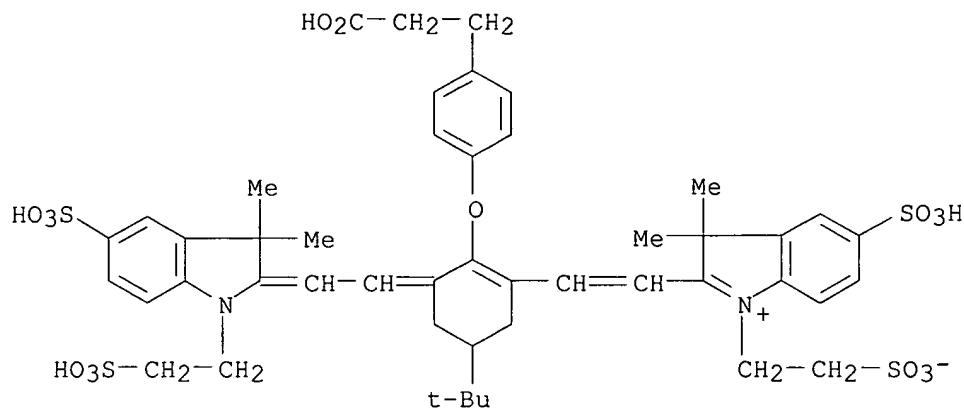
●3 Na

RN 731863-10-8 HCAPLUS
CN 3H-Indolium, 2-[4-[3-[2-[(6-aminohexyl)amino]-2-oxoethoxy]propyl]-7-[1,3-
    dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-indol-2-ylidene]-1,3,5-
    heptatrienyl]-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-, inner salt,
    trisodium salt (9CI) (CA INDEX NAME)
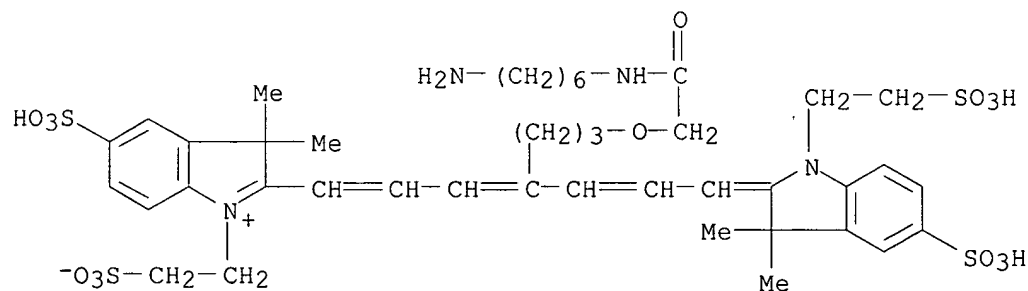
●3 Na

IT 731862-87-6P
    RL: IMF (Industrial manufacture); RCT (Reactant); RGT (Reagent); PREP
    (Preparation); RACT (Reactant or reagent)
        (manufacture of hydrophilic, thiol-reactive cyanine dyes and conjugates
        thereof with biomols. for fluorescence diagnosis)
RN 731862-87-6 HCAPLUS
CN 3H-Indolium, 2-[4-[3-[2-[[6-[(bromoacetyl)amino]hexyl]amino]-2-
    oxoethoxy]propyl]-7-[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-
    indol-2-ylidene]-1,3,5-heptatrienyl]-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-
    , inner salt, trisodium salt (9CI) (CA INDEX NAME)

$$HO_3S \quad \overset{Me}{\underset{Me}{\bigg|}} \quad CH_2-\overset{O}{\overset{\|}{C}}-NH-(CH_2)_6-NH-\overset{O}{\overset{\|}{C}}-$$

(CH2)3−O

CH=CH−CH=C−CH=CH−CH=

$^-O_3S-CH_2-CH_2$

Me

Me

SO3H

CH2−CH2−SO3H
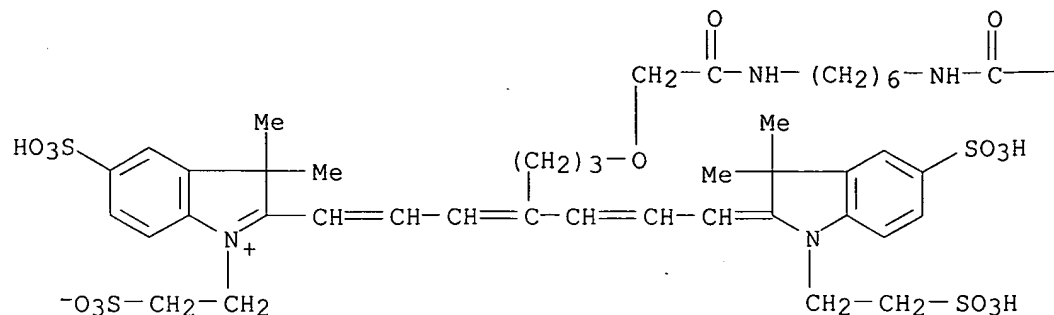
●3 Na

—CH2Br

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      731862-74-1P 731862-75-2P 731862-76-3P
      731862-77-4P 731862-78-5P 731862-79-6P
      731862-80-9P 731862-81-0P 731862-82-1P
      731862-83-2P 731862-84-3P 731862-85-4P
      731862-86-5P 731862-88-7P
      RL: IMF (Industrial manufacture); RGT (Reagent); PREP (Preparation); RACT
      (Reactant or reagent)
          (manufacture of hydrophilic, thiol-reactive cyanine dyes and conjugates
          thereof with biomols. for fluorescence diagnosis)
RN    731862-71-8  HCAPLUS
CN    3H-Indolium, 2-[7-[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-
      indol-2-ylidene]-4-[3-[[2-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-
      yl)ethyl]amino]-3-oxopropyl]-1,3,5-heptatrienyl]-3,3-dimethyl-5-sulfo-1-(2-
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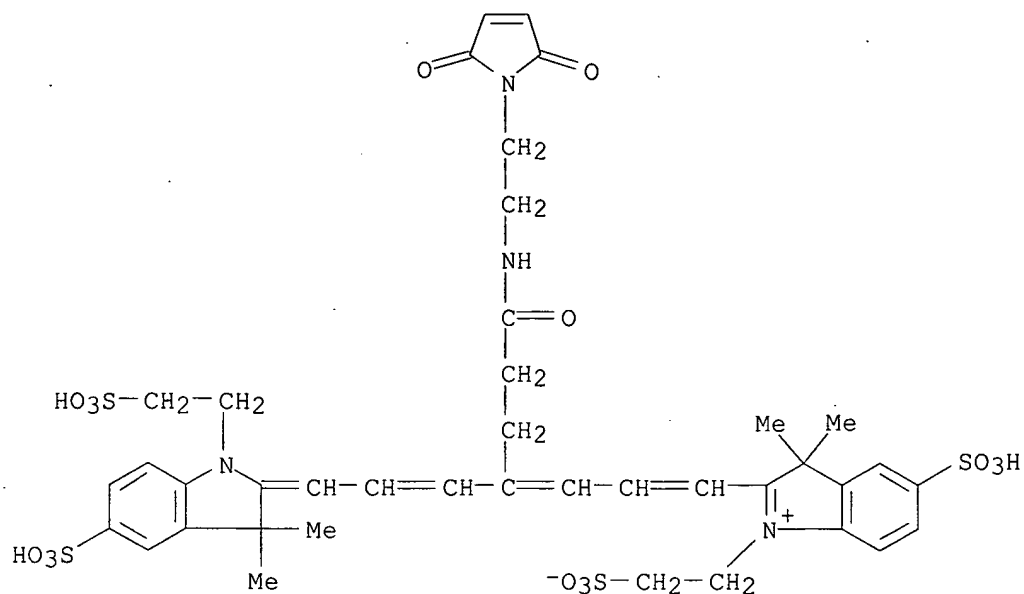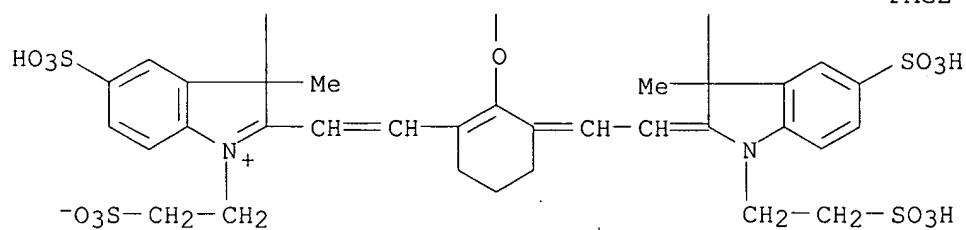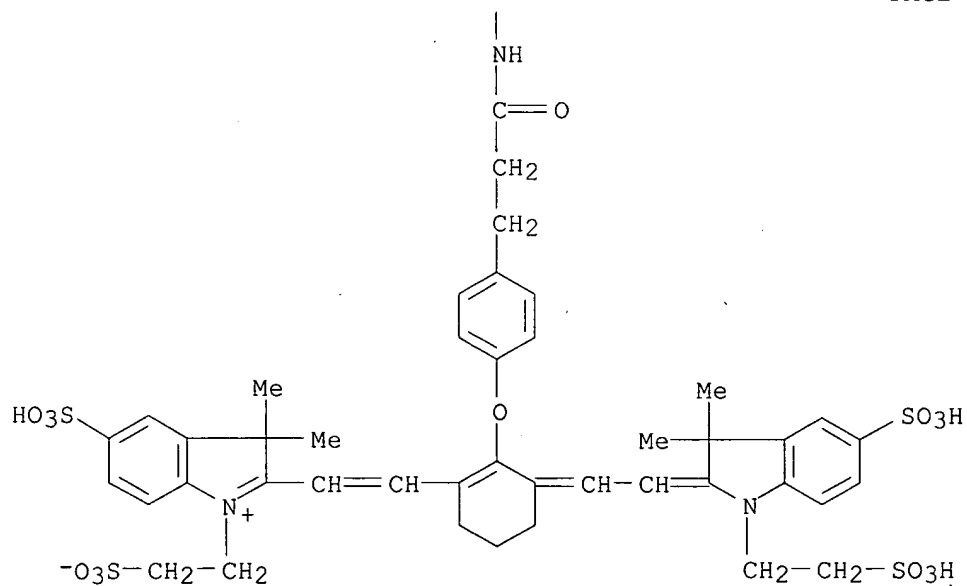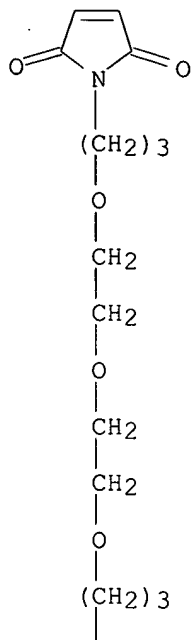
●3 Na

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      yl)hexyl]amino]-3-oxopropyl]-1,3,5-heptatrienyl]-3,3-dimethyl-5-sulfo-1-(2-
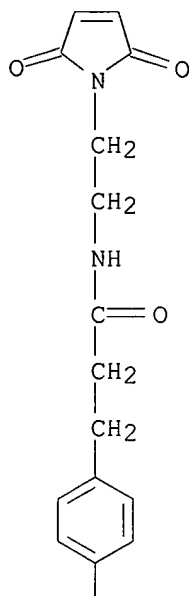   sulfoethyl)-, inner salt, trisodium salt (9CI)   (CA INDEX NAME)
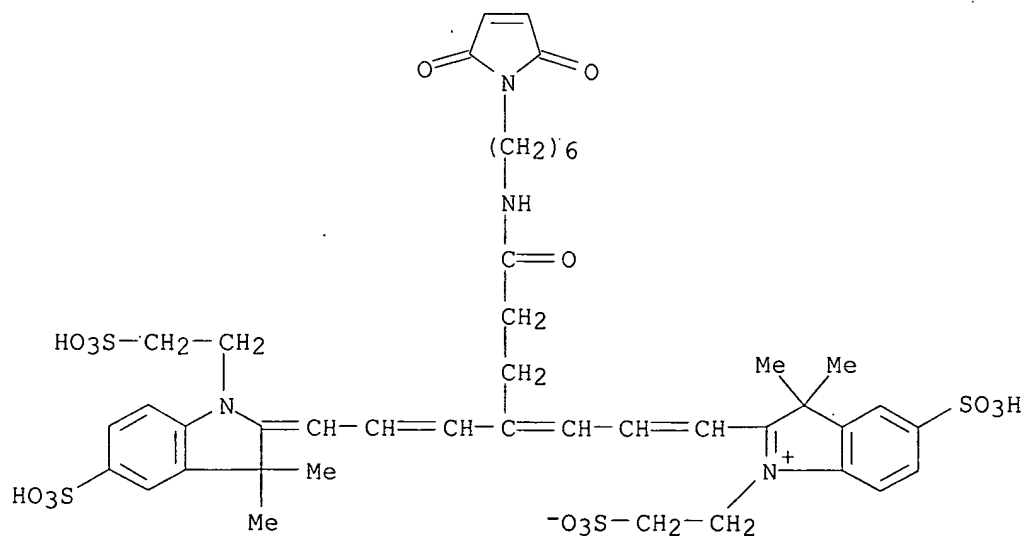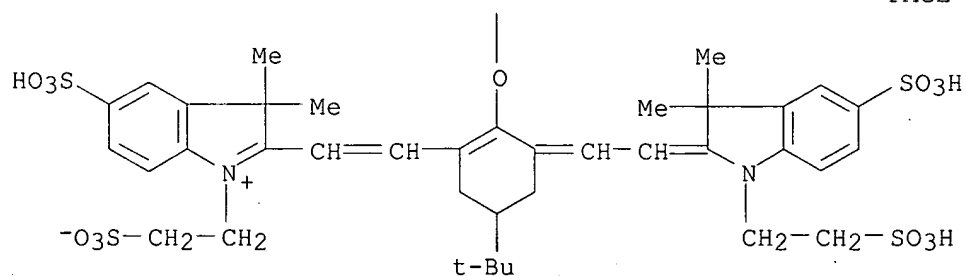
●3 Na

RN   731862-73-0 HCAPLUS
CN   3H-Indolium, 2-[4-[3-[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-
      indol-2-ylidene]-1-propenyl]-21-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)-7-
      oxo-12,15,18-trioxa-8-azaheneicosa-1,3-dien-1-yl]-3,3-dimethyl-5-sulfo-1-
      (2-sulfoethyl)-, inner salt, trisodium salt (9CI)   (CA INDEX NAME)
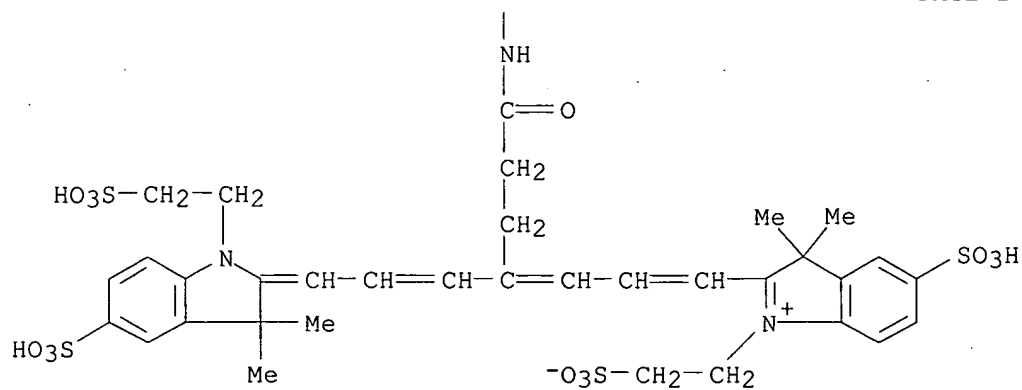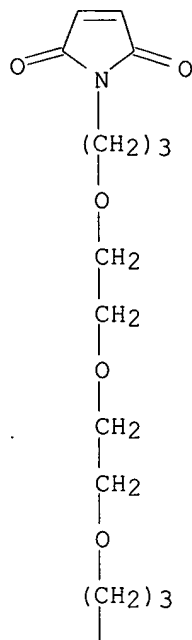
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RN   731862-74-1 HCAPLUS

CN   3H-Indolium, 2-[4-[3-[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-indol-2-ylidene]-1-propenyl]-9-[[2-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)ethyl]amino]-9-oxo-1,3-nonadienyl]-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME).

●3 Na

RN   731862-75-2 HCAPLUS

CN   3H-Indolium, 2-[4-[3-[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-indol-2-ylidene]-1-propenyl]-9-[[6-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)hexyl]amino]-9-oxo-1,3-nonadienyl]-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)

●3 Na

PAGE 1-A

PAGE 2-A

●3   Na

●3 Na

RN   731862-78-5 HCAPLUS
CN   3H-Indolium, 2-[4-[3-[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-
      indol-2-ylidene]-1-propenyl]-11-[[6-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-
      yl)hexyl]amino]-11-oxo-1,3-undecadienyl]-3,3-dimethyl-5-sulfo-1-(2-
      sulfoethyl)-, inner salt, trisodium salt (9CI)   (CA INDEX NAME)

●3 Na

RN   731862-79-6 HCAPLUS
CN   3H-Indolium, 2-[4-[3-[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-
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      oxo-16,19,22-trioxa-12-azapentacosa-1,3-dien-1-yl]-3,3-dimethyl-5-sulfo-1-
      (2-sulfoethyl)-, inner salt, trisodium salt (9CI)   (CA INDEX NAME)

(CH2)3

O

CH2

CH2

O

CH2

CH2

O

(CH2)3

NH

C=O

(CH2)6

HO3S—CH2—CH2

Me   Me

SO3H

CH=CH—CH=C—CH=CH—CH

HO3S

Me

Me

⁻O3S—CH2—CH2

●3 Na

RN 731862-80-9 HCAPLUS
CN 3H-Indolium, 2-[7-[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-
    indol-2-ylidene]-4-[3-[2-[[2-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-
    yl)ethyl]amino]-2-oxoethoxy]propyl]-1,3,5-heptatrienyl]-3,3-dimethyl-5-
    sulfo-1-(2-sulfoethyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)

●3 Na

RN   731862-81-0   HCAPLUS
CN   3H-Indolium, 2-[7-[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-
     indol-2-ylidene]-4-[3-[2-[[6-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-
     yl)hexyl]amino]-2-oxoethoxy]propyl]-1,3,5-heptatrienyl]-3,3-dimethyl-5-
     sulfo-1-(2-sulfoethyl)-, inner salt, trisodium salt (9CI)   (CA INDEX NAME)
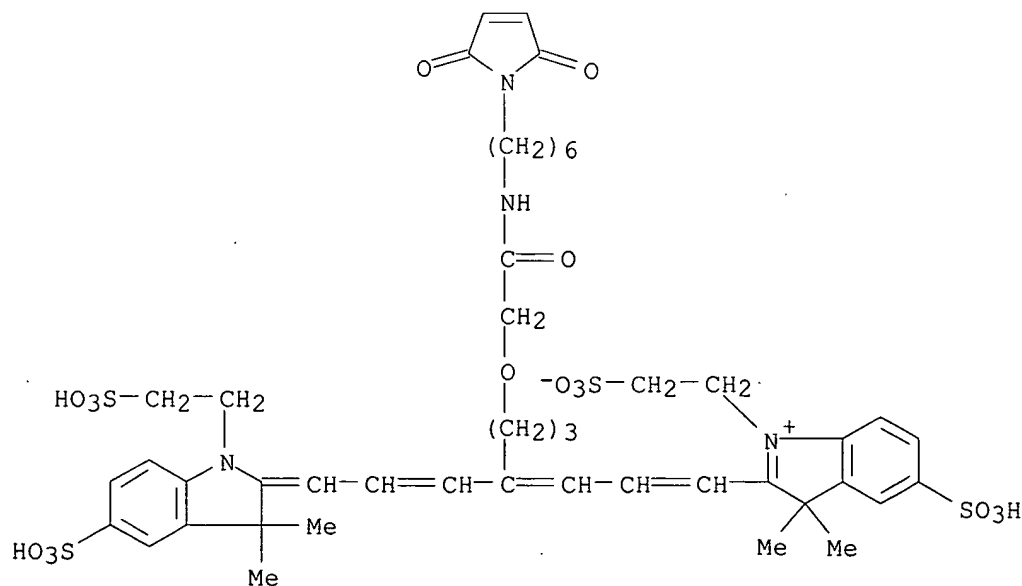
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CN   3H-Indolium, 2-[4-[3-[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-
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     oxo-8,15,18,21-tetraoxa-11-azatetracosa-1,3-dien-1-yl]-3,3-dimethyl-5-
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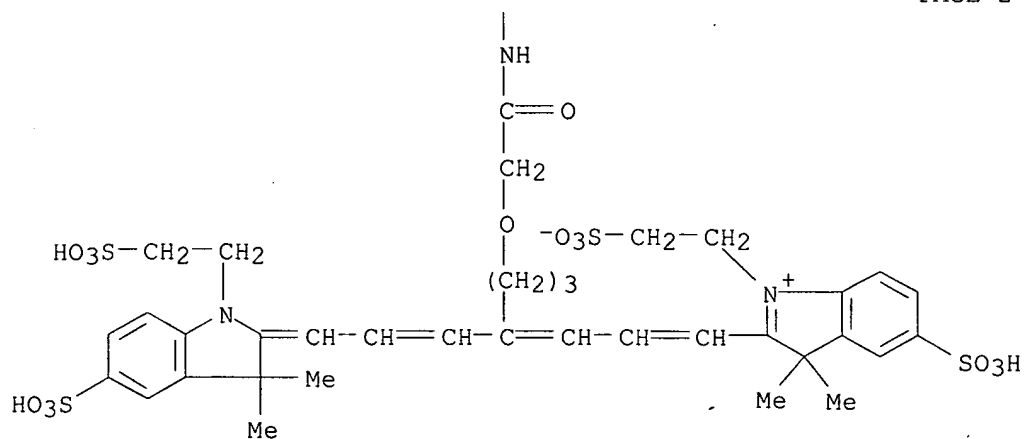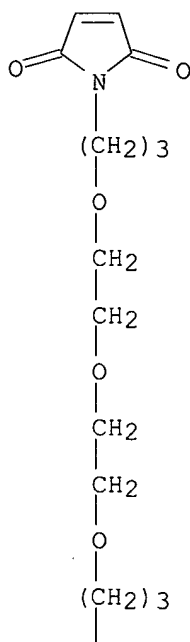
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      pyrrol-1-yl)ethyl]amino]-3-oxopropyl]phenoxy]-1-cyclohexen-1-yl]ethenyl]-
      3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-, inner salt, trisodium salt (9CI)
      (CA INDEX NAME)
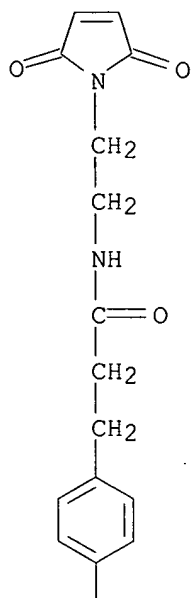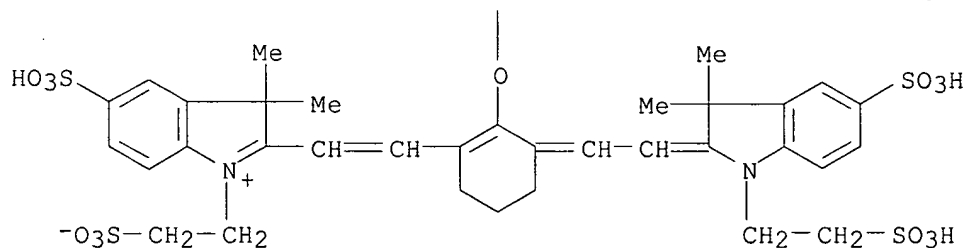
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      pyrrol-1-yl)hexyl]amino]-3-oxopropyl]phenoxy]-1-cyclohexen-1-yl]ethenyl]-
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      (CA INDEX NAME)
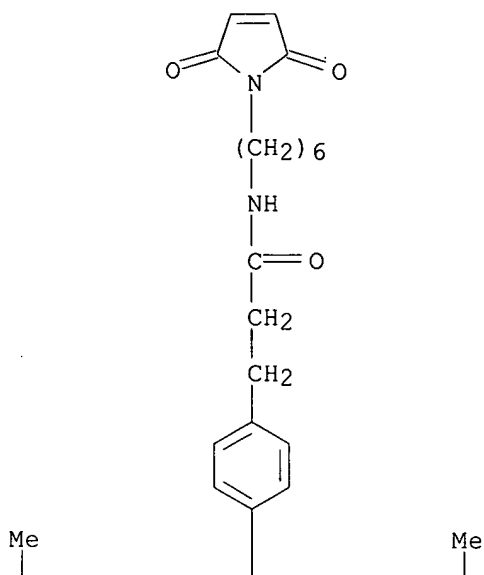
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      yl)-3-oxo-8,11,14-trioxa-4-azaheptadec-1-yl]phenoxy]-1-cyclohexen-1-
      yl]ethenyl]-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-, inner salt, trisodium
      salt (9CI) (CA INDEX NAME)

●3   Na

RN   731862-86-5   HCAPLUS
CN   3H-Indolium, 2-[2-[3-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-
     2H-indol-2-ylidene]ethylidene]-2-[4-[3-[[2-(2,5-dihydro-2,5-dioxo-1H-
     pyrrol-1-yl)ethyl]amino]-3-oxopropyl]phenoxy]-5-(1,1-dimethylethyl)-1-

cyclohexen-1-yl]ethenyl]-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-, inner
salt, trisodium salt (9CI)   (CA INDEX NAME)

●3 Na

RN   731862-88-7   HCAPLUS
CN   3H-Indolium, 2-[4-[3-[[3-[(bromoacetyl)amino]propyl]amino]-3-oxopropyl]-7-
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     1,3,5-heptatrienyl]-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-, inner salt,
     trisodium salt (9CI)   (CA INDEX NAME)
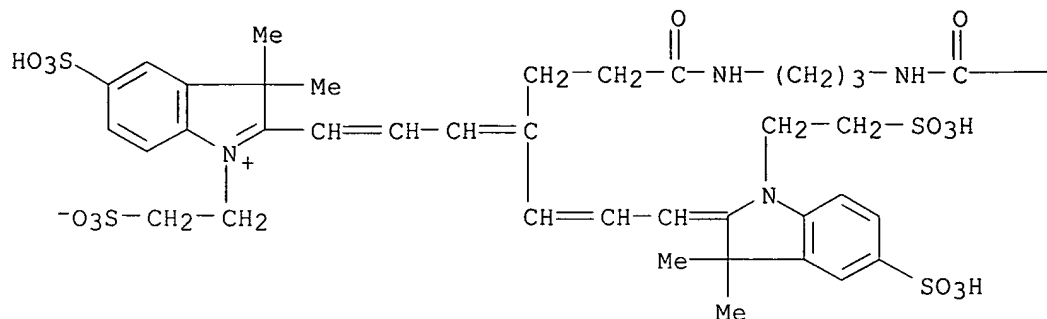
●3 Na

—CH2Br

REFERENCE COUNT: 5   THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS
                                 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 2 OF 13 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:485574 HCAPLUS
DOCUMENT NUMBER: 141:20106
TITLE: In vivo imaging of apoptosis using fluorochromes
                         conjugated to annexin A5 or synaptotagmin
INVENTOR(S):   Bogdanov, Alexei; Schellenberger, Eyk; Petrovsky,
                         Alexander; Josephson, Lee
PATENT ASSIGNEE(S):   USA
SOURCE: U.S. Pat. Appl. Publ., 24 pp.
                         CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

        PATENT NO.   KIND   DATE   APPLICATION NO.   DATE
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        US 2004022731   A1   20040205   US 2003-424232   20030425 <--
        CA 2479938   AA   20031224   CA 2003-2479938   20030428 <--
        WO 2003105814   A1   20031224   WO 2003-US13494   20030428 <--
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              GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
              LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM,
              PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT,
              TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
          RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
              KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
              FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,
   BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
        EP 1499292   A1   20050126   EP 2003-728626   20030428 <--
          R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
              IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
        JP 2005523945   T2   20050811   JP 2004-512720   20030428 <--

IT   **166547-11-1D**, IRDye-38, conjugates **398142-13-7D,**
     IRDye-78, conjugates
     RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
         (in vivo imaging of apoptosis using fluorochromes conjugated to annexin
         A5 or synaptotagmin)
RN   166547-11-1 HCAPLUS
CN   3H-Indolium, 2-[2-[3-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-
     2H-indol-2-ylidene]ethylidene]-2-(4-isothiocyanatophenoxy)-1-cyclohexen-1-
     yl]ethenyl]-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-, inner salt, trisodium
     salt (9CI) (CA INDEX NAME)

RN   398142-13-7 HCAPLUS
CN   3H-Indolium, 2-[2-[3-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-
     2H-indol-2-ylidene]ethylidene]-2-[4-[3-[(2,5-dioxo-1-pyrrolidinyl)oxy]-3-
     oxopropyl]phenoxy]-1-cyclohexen-1-yl]ethenyl]-3,3-dimethyl-5-sulfo-1-(4-
     sulfobutyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)

HO3S

Me

Me

R₁

X

N+

CH₂

CH₂

C=O

O

N

O

O

Me

Me

SO3H

N

2

CH=CH—CH=CH

R⁶

R⁷

⁻O3S—(CH₂)₄

3

(CH₂)₄—SO3H
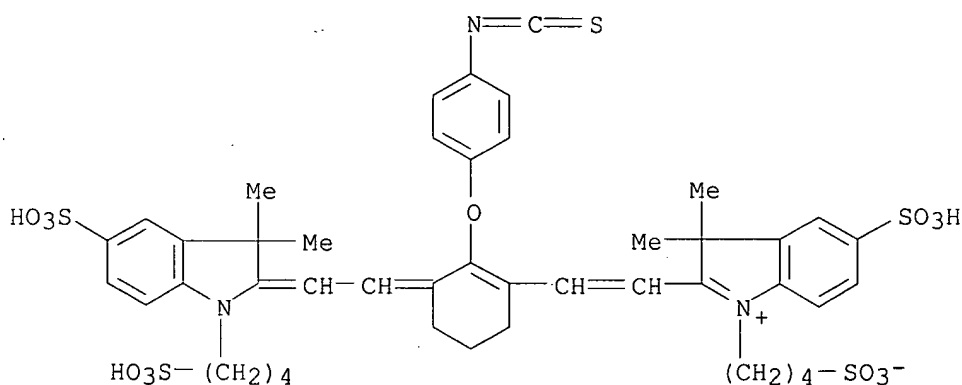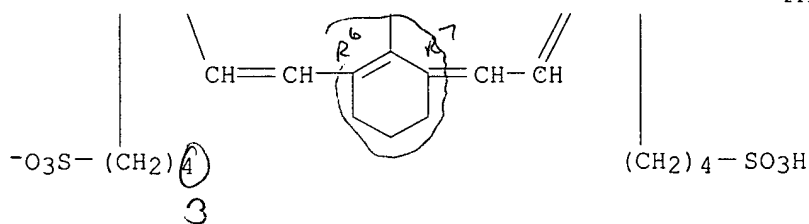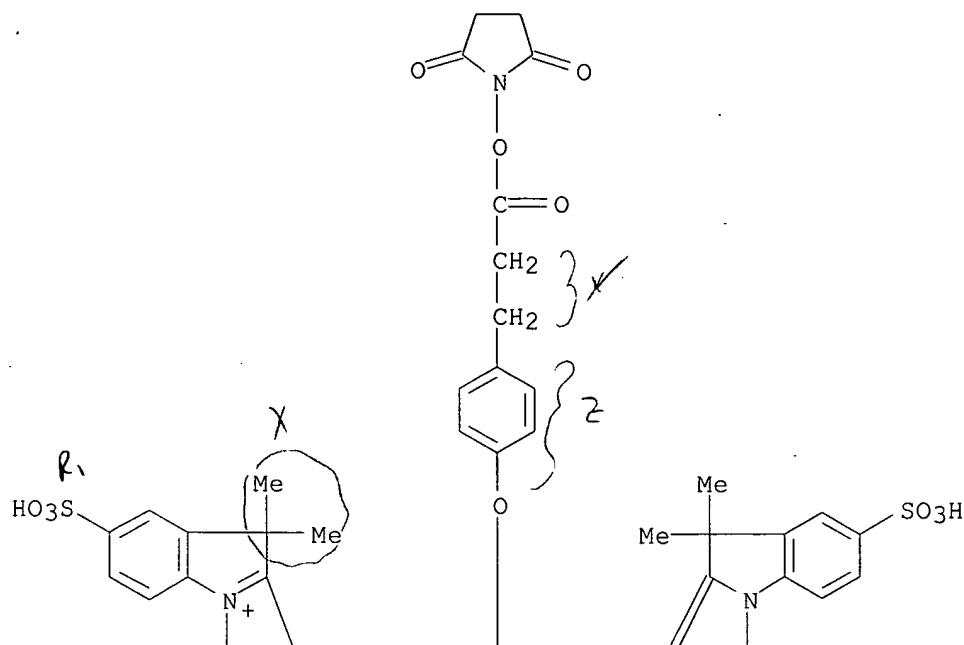
●3 Na

L32   ANSWER 3 OF 13   HCAPLUS   COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:60345   HCAPLUS
DOCUMENT NUMBER: 140:124836
TITLE: Conjugated infrared fluorescent substances for
                         detection of cell death
INVENTOR(S):   Frangioni, John V.
PATENT ASSIGNEE(S):   Beth Israel Deaconess Medical Center, USA
SOURCE: PCT Int. Appl., 68 pp.
                         CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

     PATENT NO.   KIND   DATE   APPLICATION NO.   DATE
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     WO 2004006963   A1   20040122   WO 2003-US21478   20030710 <--
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            GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,

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        LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM,
        PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN,
        TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
    RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
        KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
        FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,
        BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
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PRIORITY APPLN. INFO.:   US 2002-395582P   P 20020712 <--
OTHER SOURCE(S):   MARPAT 140:124836
IT   **166547-11-1D**, IRDye 38, conjugates with cell death-targeting agent
     RL: ARG (Analytical reagent use); BSU (Biological study, unclassified);
     DGN (Diagnostic use); ANST (Analytical study); BIOL (Biological study);
     USES (Uses)
         (IRDye 38; targeting conjugated IR fluorescent substances for detection
         of cell death)
RN   166547-11-1 HCAPLUS
CN   3H-Indolium, 2-[2-[3-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-
     2H-indol-2-ylidene]ethylidene]-2-(4-isothiocyanatophenoxy)-1-cyclohexen-1-
     yl]ethenyl]-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-, inner salt, trisodium
     salt (9CI) (CA INDEX NAME)
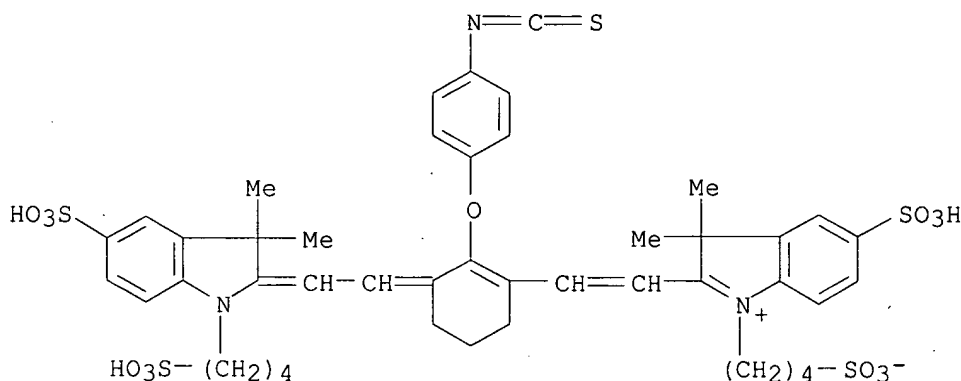
●3 Na

IT   **398142-13-7D**, IRDye 78, conjugates with annexin V
     RL: ARG (Analytical reagent use); BSU (Biological study, unclassified);
     DGN (Diagnostic use); ANST (Analytical study); BIOL (Biological study);
     USES (Uses)
         (targeting conjugated IR fluorescent substances for detection of cell
         death)
RN   398142-13-7 HCAPLUS
CN   3H-Indolium, 2-[2-[3-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-
     2H-indol-2-ylidene]ethylidene]-2-[4-[3-[(2,5-dioxo-1-pyrrolidinyl)oxy]-3-
     oxopropyl]phenoxy]-1-cyclohexen-1-yl]ethenyl]-3,3-dimethyl-5-sulfo-1-(4-
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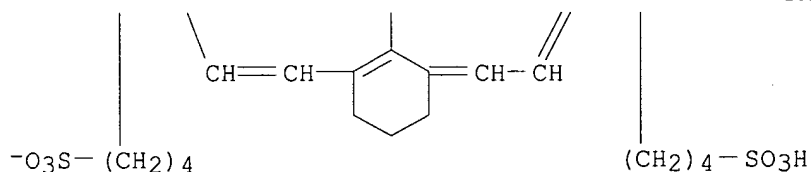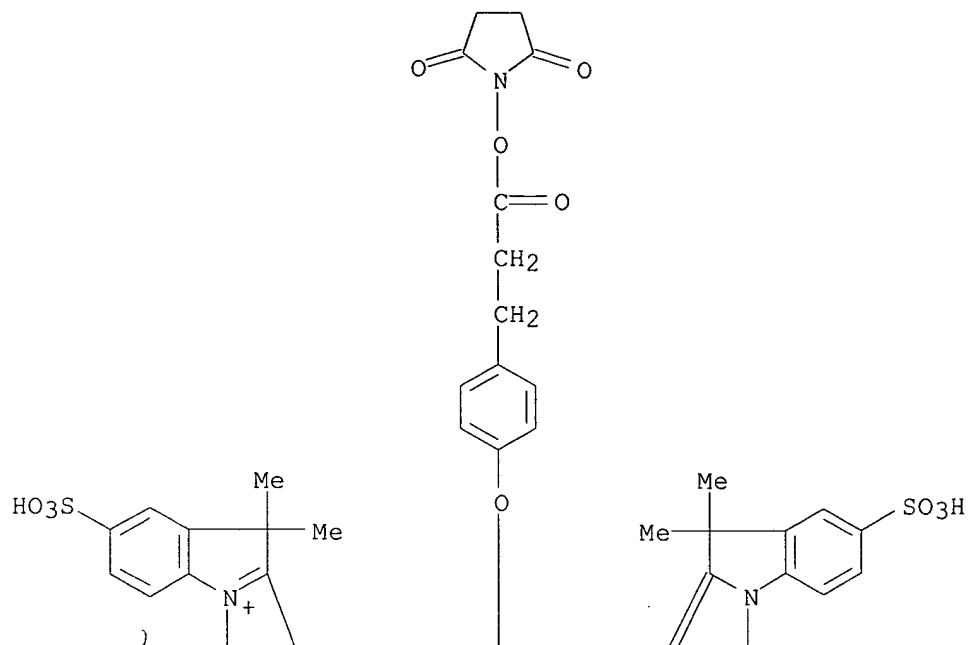
● 3 Na

REFERENCE COUNT: 5   THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS
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L32 ANSWER 4 OF 13 HCAPLUS   COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2003:470344 HCAPLUS
DOCUMENT NUMBER: 139:48112
TITLE: High throughput analysis and detection of multiple
                         target nucleotide sequences such as single nucleotide
                         polymorphisms
INVENTOR(S):   Van Eijk, Michael J. T.
PATENT ASSIGNEE(S):   Keygene N.V., Neth.
SOURCE: Eur. Pat. Appl., 63 pp.
                         CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

        PATENT NO.   KIND   DATE   APPLICATION NO.   DATE
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        EP 1319718   A1   20030618   EP 2001-204912   20011214

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          GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
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PRIORITY APPLN. INFO.:                        EP 2001-204912      A    20011214 <--
                                              WO 2002-NL834       W    20021216 <--
IT   398142-13-7D, oligonucleotide conjugates
     RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
         (IRDye; high throughput anal. and detection of multiple target
         nucleotide sequences such as single nucleotide polymorphisms)
RN   398142-13-7 HCAPLUS
CN   3H-Indolium, 2-[2-[3-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-
     2H-indol-2-ylidene]ethylidene]-2-[4-[3-[(2,5-dioxo-1-pyrrolidinyl)oxy]-3-
     oxopropyl]phenoxy]-1-cyclohexen-1-yl]ethenyl]-3,3-dimethyl-5-sulfo-1-(4-
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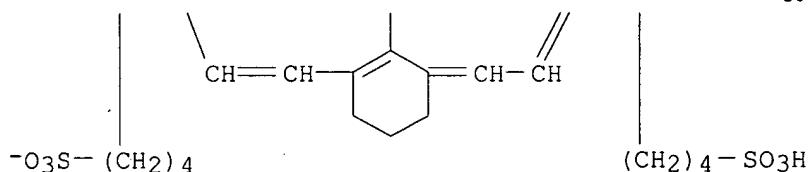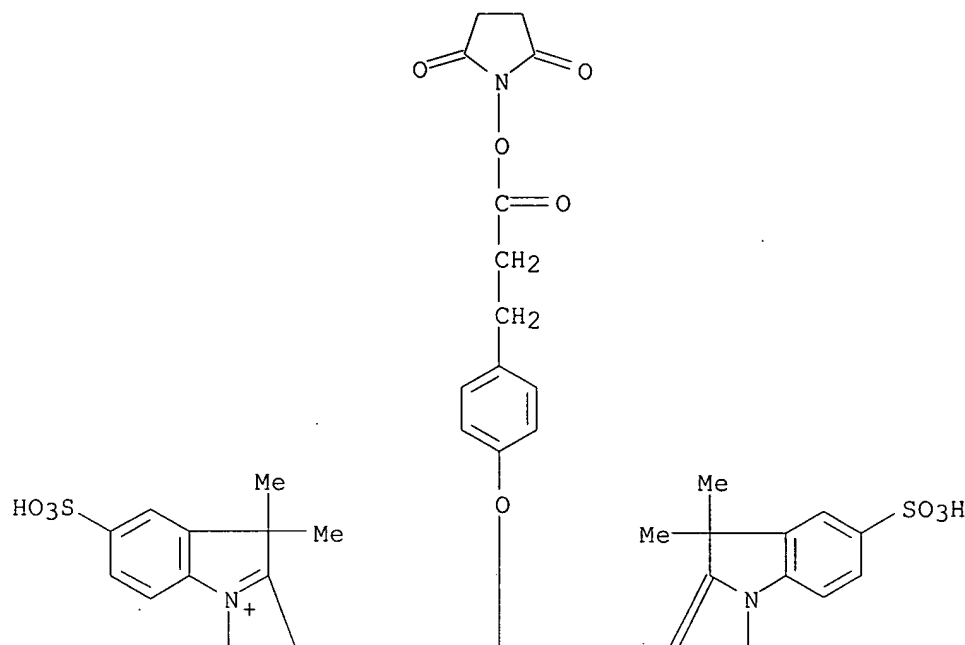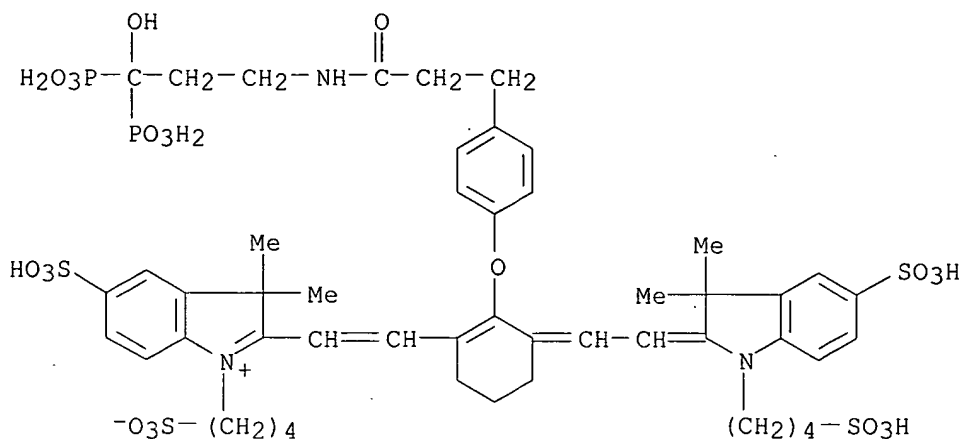
●3 Na

REFERENCE COUNT: 8   THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS
                                  RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RN   607709-66-0   HCAPLUS
CN   3H-Indolium, 2-[2-[3-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-
      2H-indol-2-ylidene]ethylidene]-2-[4-[3-[(2-hydroxyethyl)amino]-3-
      oxopropyl]phenoxy]-1-cyclohexen-1-yl]ethenyl]-3,3-dimethyl-5-sulfo-1-(4-
      sulfobutyl)-, inner salt, compd. with N,N-diethylethanamine (1:3) (9CI)
   (CA INDEX NAME)

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      CRN   607709-65-9
      CMF   C49 H61 N3 O15 S4

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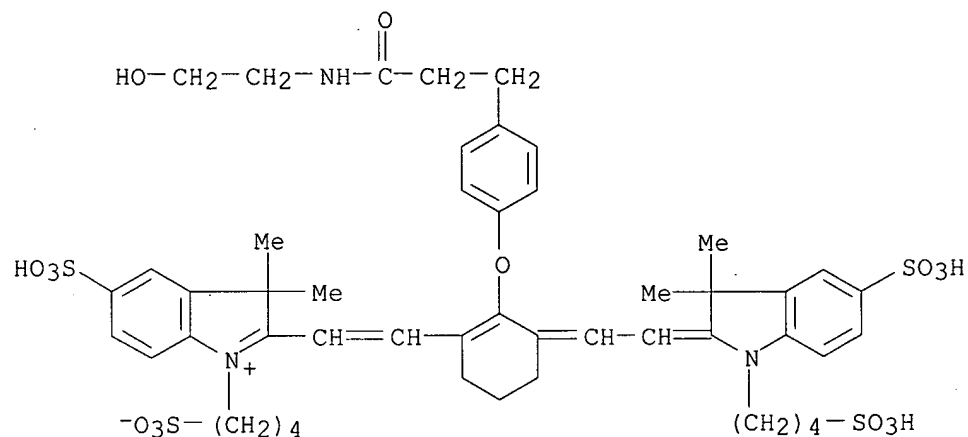
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      CMF   C6 H15 N
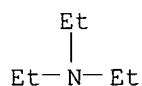
RN   607709-68-2   HCAPLUS
CN   3H-Indolium, 2-[2-[2-[4-[3-[[(1S)-4-[(aminoiminomethyl)amino]-1-
      formylbutyl]amino]-3-oxopropyl]phenoxy]-3-[[1,3-dihydro-3,3-dimethyl-5-
      sulfo-1-(4-sulfobutyl)-2H-indol-2-ylidene]ethylidene]-1-cyclohexen-1-
      yl]ethenyl]-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-, inner salt, compd.
      with N,N-diethylethanamine (1:3) (9CI)   (CA INDEX NAME)

      CM   1

      CRN   607709-67-1
      CMF   C53 H68 N6 O15 S4

Absolute stereochemistry.
Double bond geometry unknown.
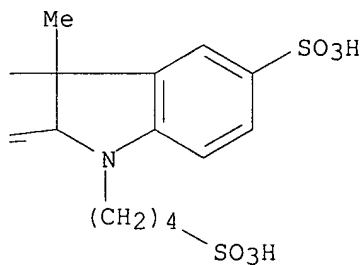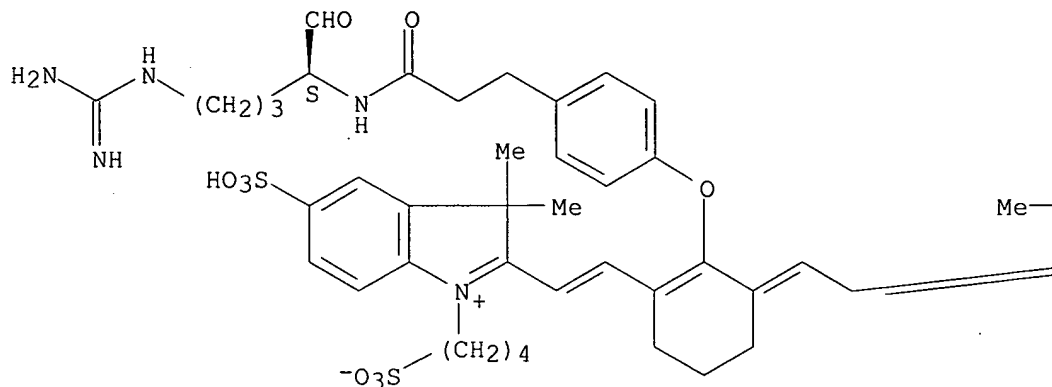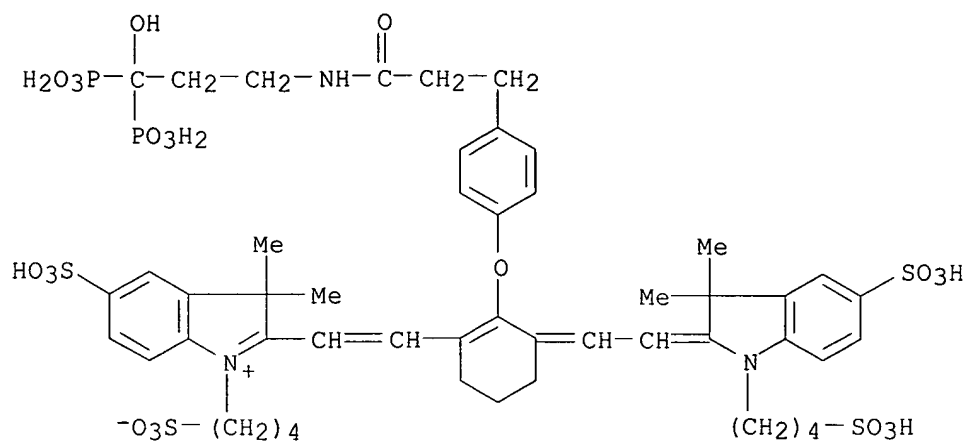
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CM      2

CRN     121-44-8
CMF     C6 H15 N
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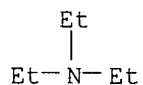


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RN      607709-70-6  HCAPLUS
CN      3H-Indolium, 2-[2-[2-[4-[3-[[(1S)-3-carboxy-1-formylpropyl]amino]-3-
        oxopropyl]phenoxy]-3-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-
        2H-indol-2-ylidene]ethylidene]-1-cyclohexen-1-yl]ethenyl]-3,3-dimethyl-5-
        sulfo-1-(4-sulfobutyl)-, inner salt, compd. with N,N-diethylethanamine
        (1:3) (9CI)  (CA INDEX NAME)

CM      1

CRN     607709-69-3
CMF     C52 H63 N3 O17 S4

Absolute stereochemistry.
Double bond geometry unknown.
```

─SO3H

```
    CM    2

    CRN   121-44-8
    CMF   C6 H15 N
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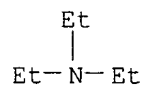


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RN    607709-72-8   HCAPLUS
CN    L-Glutamic acid, N-[3-[4-[[6-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(4-
      sulfobutyl)-2H-indol-2-ylidene]ethylidene]-2-[2-[3,3-dimethyl-5-sulfo-1-(4-
      sulfobutyl)-3H-indolium-2-yl]ethenyl]-1-cyclohexen-1-yl]oxy]phenyl]-1-
      oxopropyl]-L-β-aspartyl-, inner salt, compd. with
      N,N-diethylethanamine (1:3) (9CI)    (CA INDEX NAME)

    CM    1

    CRN   607709-71-7
    CMF   C56 H68 N4 O21 S4
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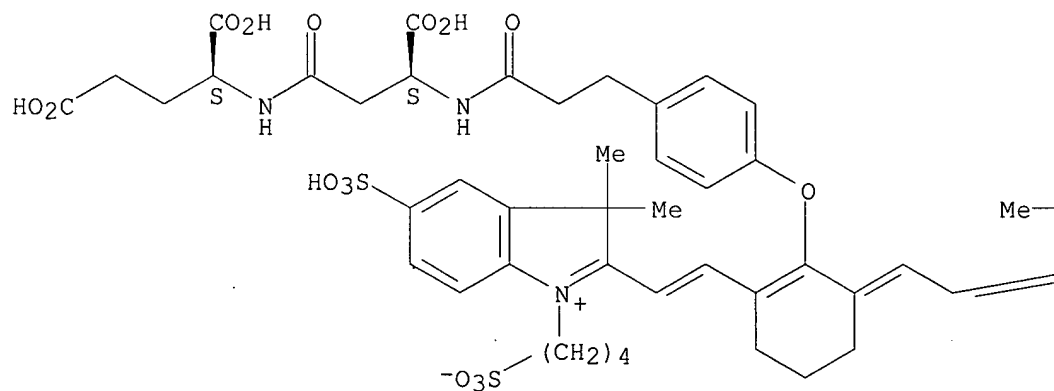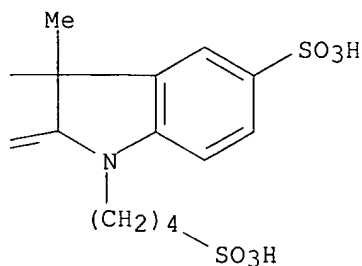
Absolute stereochemistry.
Double bond geometry unknown.
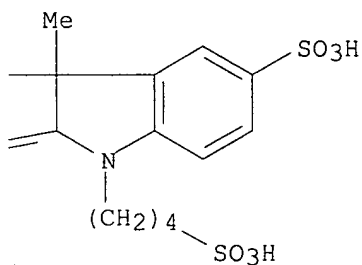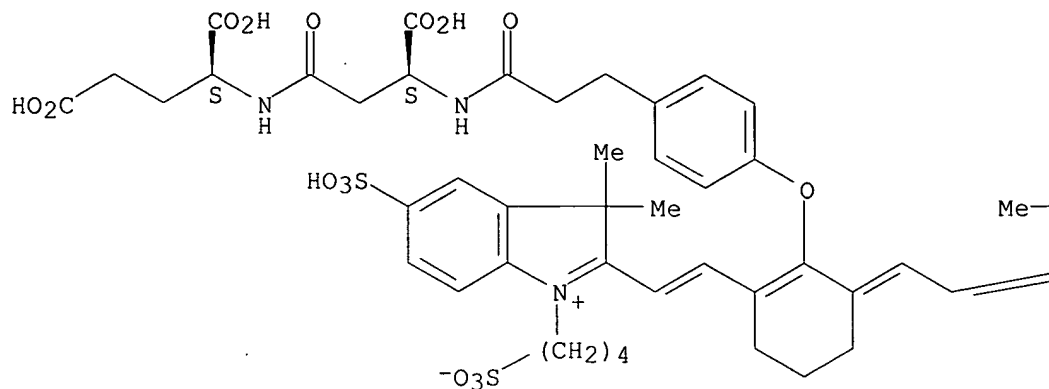
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        CM    2

        CRN   121-44-8
        CMF   C6 H15 N
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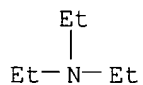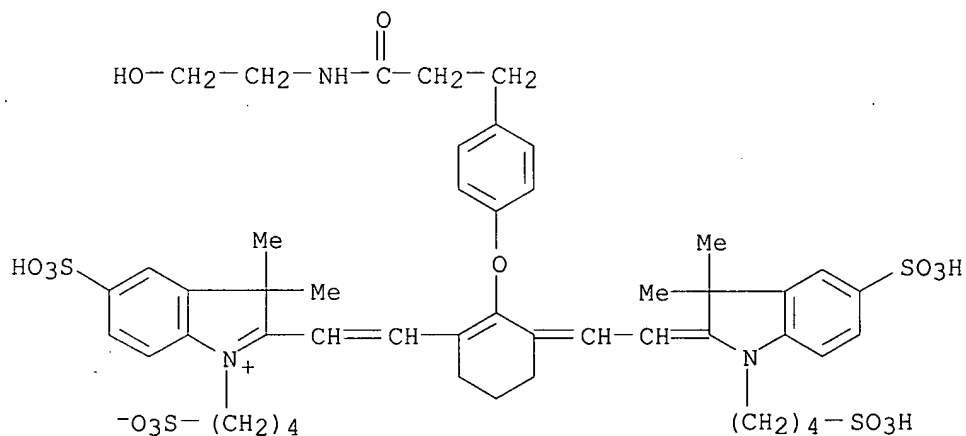


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CN   3H-Indolium, 2-[2-[3-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-
     2H-indol-2-ylidene]ethylidene]-2-[4-[3-[(3-hydroxy-3,3-
     diphosphonopropyl)amino]-3-oxopropyl]phenoxy]-1-cyclohexen-1-yl]ethenyl]-
     3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-, inner salt, compd. with
     N,N-diethylethanamine (1:7) (9CI)  (CA INDEX NAME)

     CM    1

     CRN   607709-73-9
     CMF   C50 H65 N3 O21 P2 S4
```

H2O3P–C–CH2–CH2–NH–C–CH2–CH2
OH
PO3H2
O

(structure: cyanine dye with indolium systems)

HO3S ... Me Me ... Me Me ... SO3H

CH=CH ... CH–CH=

N+ ... N

⁻O3S—(CH2)4 ... (CH2)4—SO3H

CM   2

CRN   121-44-8
CMF   C6 H15 N

Et
|
Et— N— Et
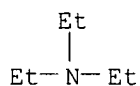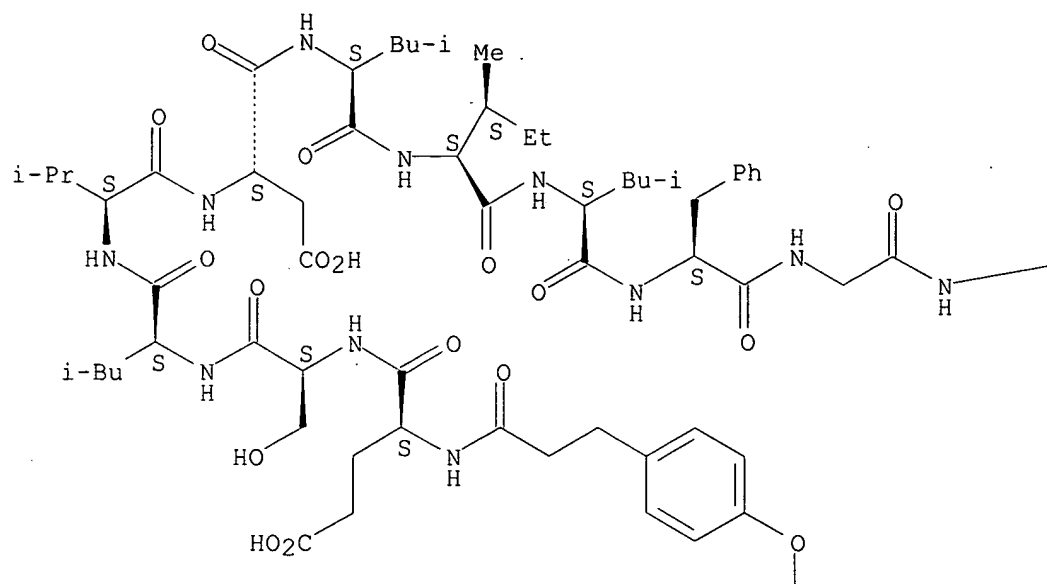
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      2H-indol-2-ylidene]ethylidene]-2-[2-[3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-
      3H-indolium-2-yl]ethenyl]-1-cyclohexen-1-yl]oxy]phenyl]-1-oxopropyl]-L-
      α-glutamyl-L-seryl-L-leucyl-L-valyl-L-α-aspartyl-L-leucyl-L-
      isoleucyl-L-leucyl-L-phenylalanylglycyl-, inner salt, compd. with
      N,N-diethylethanamine (1:7) (9CI)   (CA INDEX NAME)

CM   1

CRN   607709-75-1
CMF   C102 H143 N13 O32 S4

Absolute stereochemistry.
Double bond geometry unknown.

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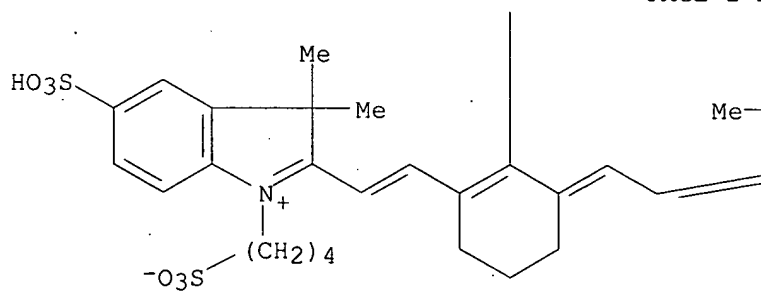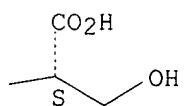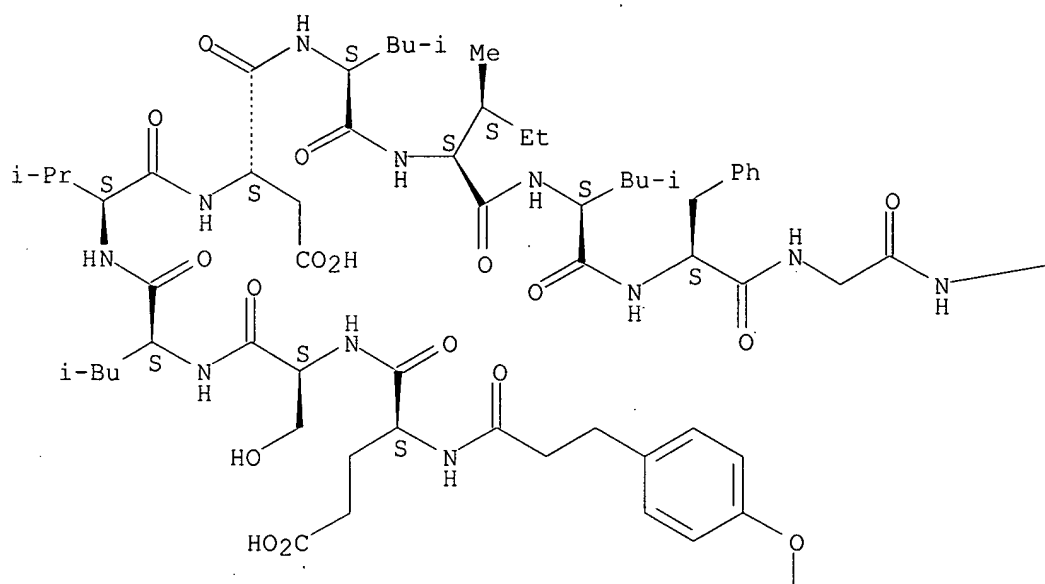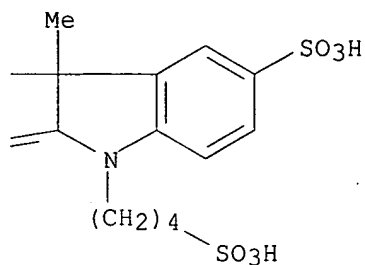
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CMF   C6 H15 N
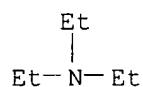
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      yl)ethyl]amino]-3-oxopropyl]phenoxy]-1-cyclohexen-1-yl]ethenyl]-3,3-
      dimethyl-5-sulfo-1-(4-sulfobutyl)-, inner salt, compd. with
      N,N-diethylethanamine (1:3) (9CI)   (CA INDEX NAME)

      CM   1

      CRN   607709-77-3
      CMF   C58 H66 N4 O15 S4

Absolute stereochemistry.
Double bond geometry unknown.

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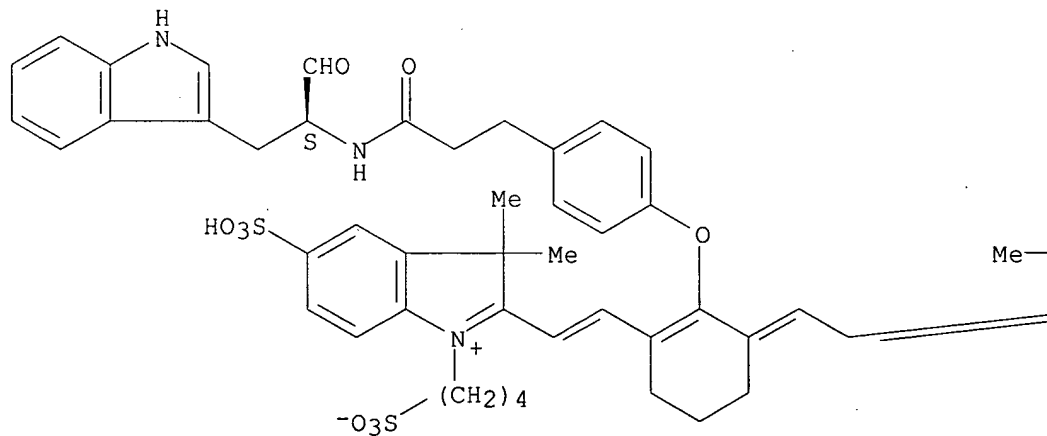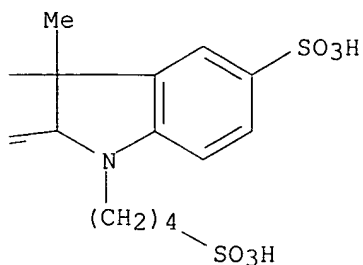
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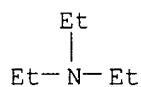
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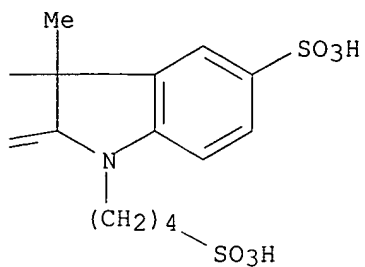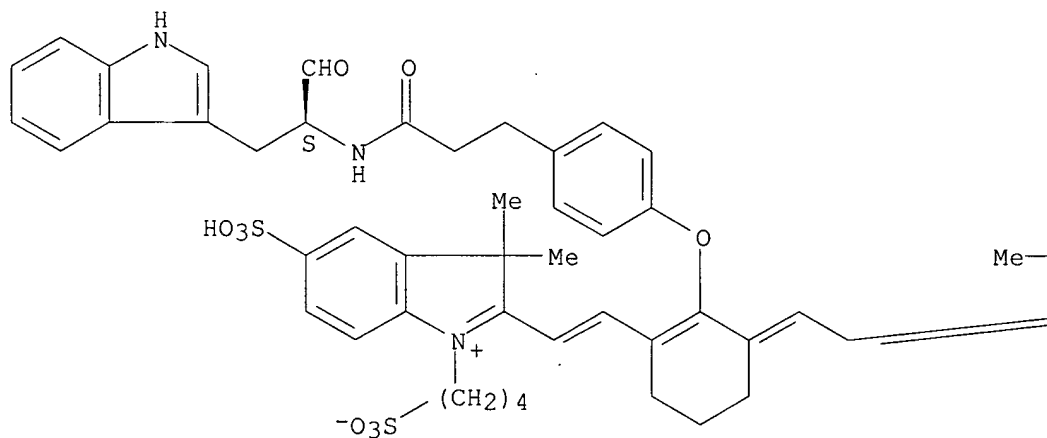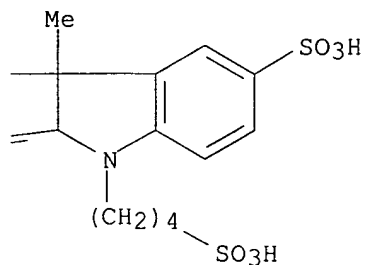RN   397858-89-8 HCAPLUS
CN   3H-Indolium, 2-[2-[3-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-
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      diphosphonopropyl)amino]-3-oxopropyl]phenoxy]-1-cyclohexen-1-yl]ethenyl]-
      3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-, inner salt, heptasodium salt (9CI)
         (CA INDEX NAME)

(Top chemical structure)

OH

H2O3P—C—CH2—CH2—NH—C(=O)—CH2—CH2

PO3H2

HO3S ... Me Me ... SO3H

CH=CH ... CH=CH

N+ ... N

‾O3S—(CH2)4 ... (CH2)4—SO3H

● 7 Na

RN   477808-86-9   HCAPLUS
CN   L-Glutamic acid, N-[3-[4-[[6-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(4-
     sulfobutyl)-2H-indol-2-ylidene]ethylidene]-2-[2-[3,3-dimethyl-5-sulfo-1-(4-
     sulfobutyl)-3H-indolium-2-yl]ethenyl]-1-cyclohexen-1-yl]oxy]phenyl]-1-
     oxopropyl]-L-β-aspartyl-, inner salt, trisodium salt (9CI)   (CA INDEX
     NAME)

Absolute stereochemistry.
Double bond geometry unknown.

(Bottom chemical structure)

CO2H   O   CO2H   O

HO2C ... S ... N ... S ... N ... Me

H ... H

HO3S ... Me Me ... O

N+ ... CH=CH

‾O3S ... (CH2)4 ... Me—

● 3 Na

RN   607709-59-1   HCAPLUS
CN   3H-Indolium, 2-[2-[3-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-
      2H-indol-2-ylidene]ethylidene]-2-[4-[3-[(2-hydroxyethyl)amino]-3-
      oxopropyl]phenoxy]-1-cyclohexen-1-yl]ethenyl]-3,3-dimethyl-5-sulfo-1-(4-
      sulfobutyl)-, inner salt, trisodium salt (9CI)   (CA INDEX NAME)

● 3   Na

RN   607709-60-4   HCAPLUS
CN   3H-Indolium, 2-[2-[2-[4-[3-[[(1S)-4-[(aminoiminomethyl)amino]-1-
      formylbutyl]amino]-3-oxopropyl]phenoxy]-3-[[1,3-dihydro-3,3-dimethyl-5-
      sulfo-1-(4-sulfobutyl)-2H-indol-2-ylidene]ethylidene]-1-cyclohexen-1-
      yl]ethenyl]-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-, inner salt, trisodium
      salt (9CI)   (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.
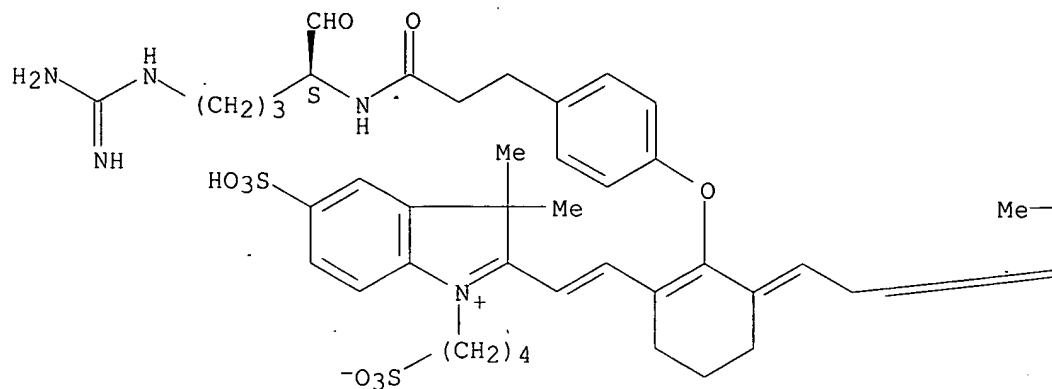
●3 Na
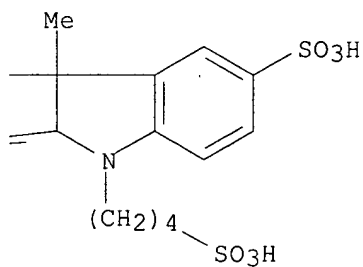
RN   607709-61-5   HCAPLUS
CN   3H-Indolium, 2-[2-[2-[4-[3-[[(1S)-3-carboxy-1-formylpropyl]amino]-3-
      oxopropyl]phenoxy]-3-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-
      2H-indol-2-ylidene]ethylidene]-1-cyclohexen-1-yl]ethenyl]-3,3-dimethyl-5-
      sulfo-1-(4-sulfobutyl)-, inner salt, trisodium salt (9CI)   (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.
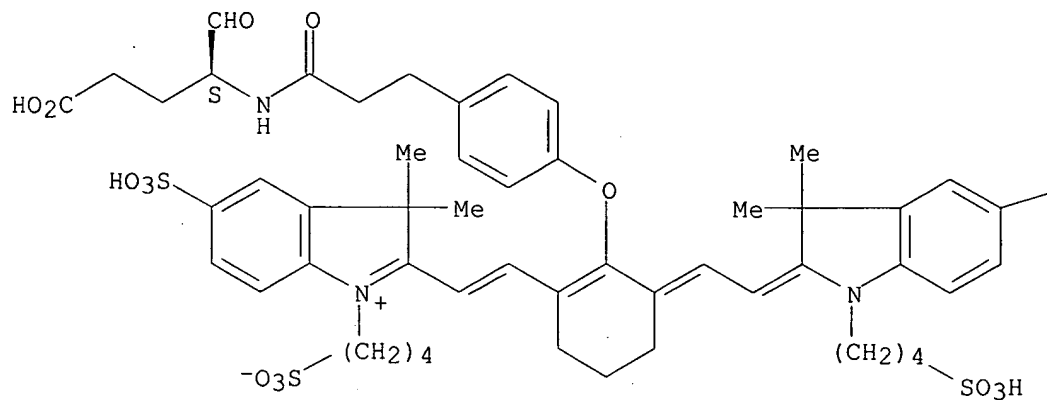
3 Na

—SO3H

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RN   607709-63-7   HCAPLUS
CN   L-Serine, N-[3-[4-[[6-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-
     2H-indol-2-ylidene]ethylidene]-2-[2-[3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-
     3H-indolium-2-yl]ethenyl]-1-cyclohexen-1-yl]oxy]phenyl]-1-oxopropyl]-L-
     α-glutamyl-L-seryl-L-leucyl-L-valyl-L-α-aspartyl-L-leucyl-L-
     isoleucyl-L-leucyl-L-phenylalanylglycyl-, inner salt, trisodium salt (9CI)
       (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.
```

Absolute stereochemistry.
Double bond geometry unknown.

●3 Na

IT · **398142-13-7**
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (purification of IRDye78 conjugates by ion-pairing HPLC in relation to
        applications for near-IR fluorescence imaging)
RN   398142-13-7 HCAPLUS
CN   3H-Indolium, 2-[2-[3-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-
     2H-indol-2-ylidene]ethylidene]-2-[4-[3-[(2,5-dioxo-1-pyrrolidinyl)oxy]-3-
     oxopropyl]phenoxy]-1-cyclohexen-1-yl]ethenyl]-3,3-dimethyl-5-sulfo-1-(4-
   sulfobutyl)-, inner salt, trisodium salt (9CI)   (CA INDEX NAME)

$$^-O_3S-(CH_2)_4 \qquad CH=CH-\!\!\!\!\bigcirc\!\!\!\!=CH-CH \qquad (CH_2)_4-SO_3H$$
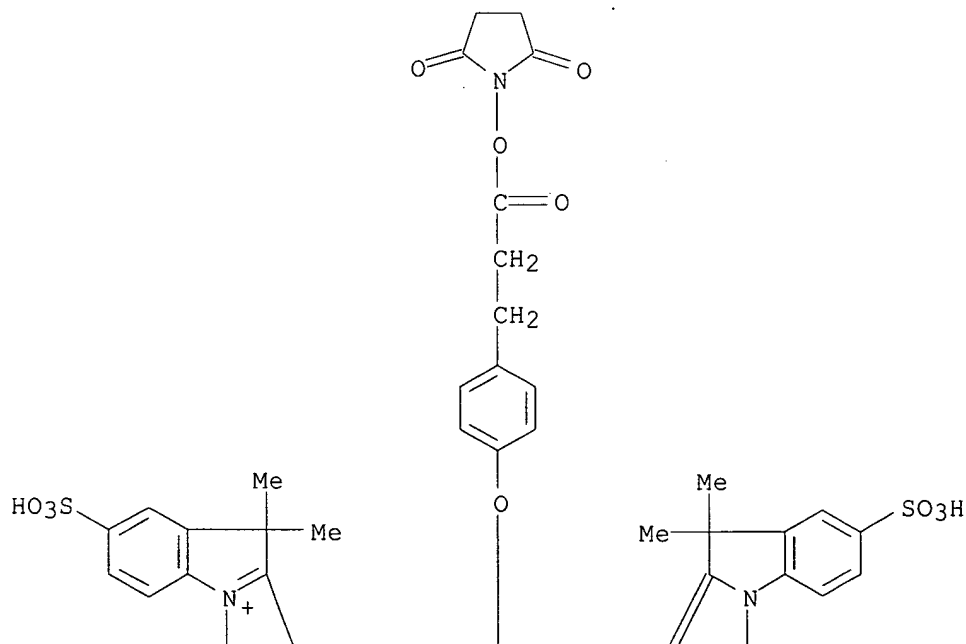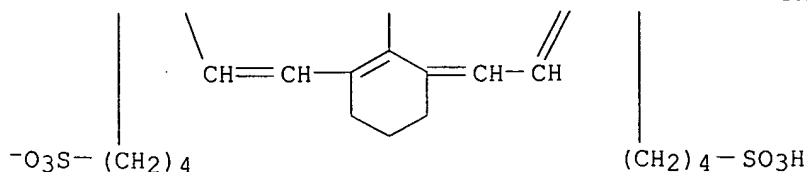
●3 Na

REFERENCE COUNT: 15   THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS
                               RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 6 OF 13 HCAPLUS   COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:946293 HCAPLUS
DOCUMENT NUMBER: 138:19479
TITLE: Modified PSMA ligands for diagnosis and treatment of
                            prostate cancer
INVENTOR(S):   Frangioni, John V.
PATENT ASSIGNEE(S):   Beth Israel Deaconess Medical Center, USA
SOURCE: PCT Int. Appl., 72 pp.
                            CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

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        PATENT NO.            KIND   DATE       APPLICATION NO.        DATE
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        WO 2002098885         A1     20021212   WO 2002-US21996        20020207 <--
            W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
                CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM,
                HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS,
                LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO,
                RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ,
                VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
            RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH,
                CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,
                BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
        CA 2436408            AA     20021212   CA 2002-2436408        20020207 <--
        EP 1363920            A1     20031126   EP 2002-761082         20020207 <--
            R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
                IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
        US 2004110723         A1     20040610   US 2002-71890          20020207 <--
        US 6875886            B2     20050405
        JP 2005507857         T2     20050324   JP 2003-502006         20020207 <--
        US 2004229845         A1     20041118   US 2004-869790         20040616 <--
PRIORITY APPLN. INFO.:                          US 2001-267055P      P  20010207 <--
                                                US 2002-71890        A1 20020207 <--
                                                WO 2002-US21996      W  20020207 <--
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OTHER SOURCE(S):   MARPAT 138:19479
IT   **398142-13-7**, IRDye78
      RL: BSU (Biological study, unclassified); BIOL (Biological study)
         (modified PSMA ligands for diagnosis and treatment of prostate cancer)
RN   398142-13-7 HCAPLUS
CN   3H-Indolium, 2-[2-[3-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-
      2H-indol-2-ylidene]ethylidene]-2-[4-[3-[(2,5-dioxo-1-pyrrolidinyl)oxy]-3-
      oxopropyl]phenoxy]-1-cyclohexen-1-yl]ethenyl]-3,3-dimethyl-5-sulfo-1-(4-
      sulfobutyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)

●3 Na
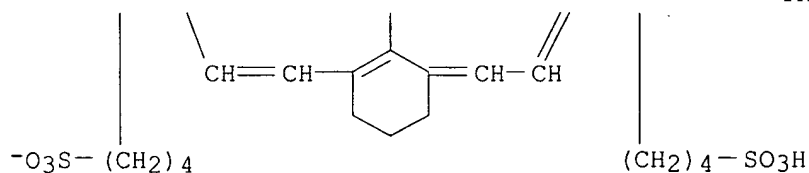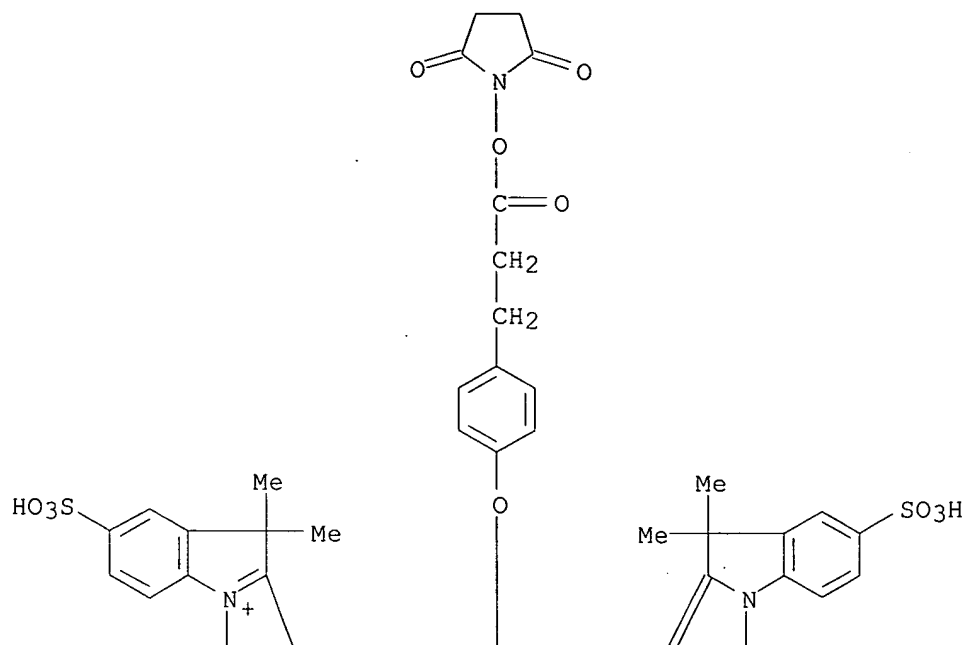
IT   **477808-85-8 477808-86-9**
     RL: DGN (Diagnostic use); BIOL (Biological study); USES (Uses)
     (modified PSMA ligands for diagnosis and treatment of prostate cancer)
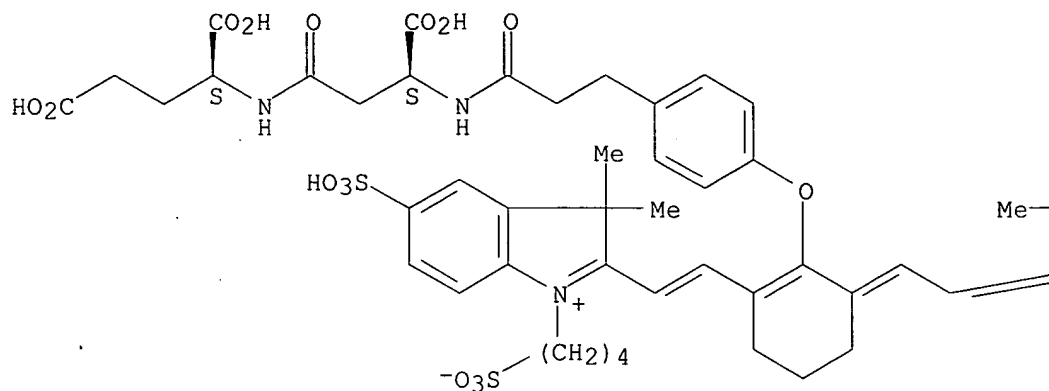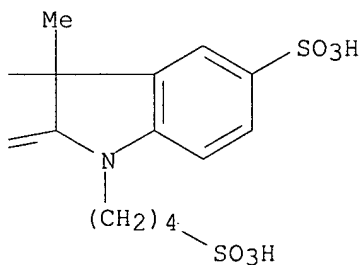RN   477808-85-8   HCAPLUS
CN   3H-Indolium, 2-[2-[2-[4-[3-[[1-carboxy-3-[(2,4-
     dicarboxybutyl)hydroxyphosphinyl]propyl]amino]-3-oxopropyl]phenoxy]-3-
     [[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-2H-indol-2-
     ylidene]ethylidene]-1-cyclohexen-1-yl]ethenyl]-3,3-dimethyl-5-sulfo-1-(4-
     sulfobutyl)-, inner salt, trisodium salt (9CI)   (CA INDEX NAME)
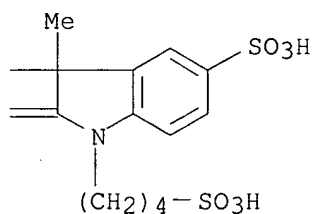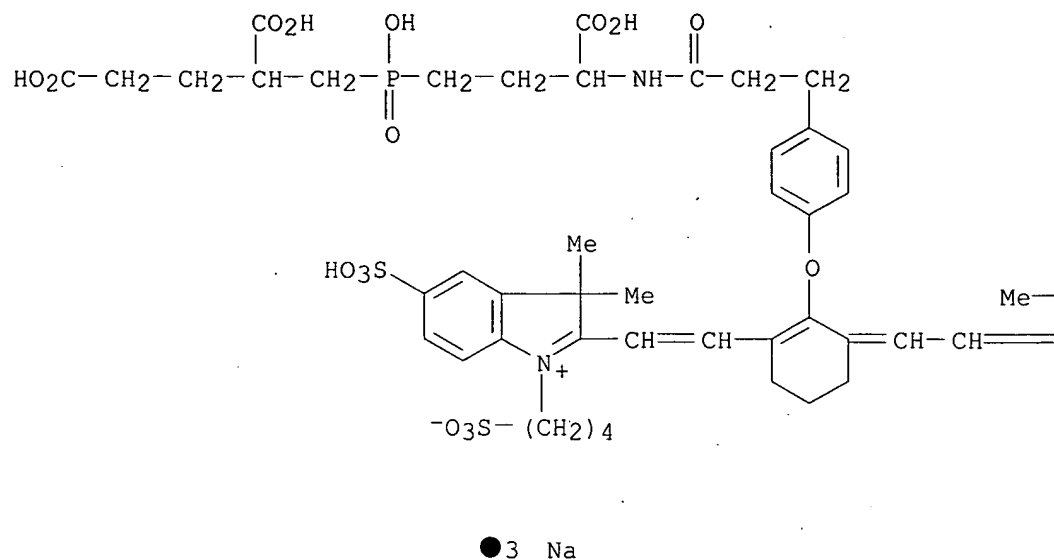
RN   477808-86-9 HCAPLUS
CN   L-Glutamic acid, N-[3-[4-[[6-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(4-
      sulfobutyl)-2H-indol-2-ylidene]ethylidene]-2-[2-[3,3-dimethyl-5-sulfo-1-(4-
      sulfobutyl)-3H-indolium-2-yl]ethenyl]-1-cyclohexen-1-yl]oxy]phenyl]-1-
      oxopropyl]-L-β-aspartyl-, inner salt, trisodium salt (9CI) (CA INDEX
      NAME)

Absolute stereochemistry.
Double bond geometry unknown.

● 3 Na

REFERENCE COUNT: 2   THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS
                                 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 7 OF 13 HCAPLUS   COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:368351 HCAPLUS
DOCUMENT NUMBER: 136:366118
TITLE: Non-isotopic detection of osteoblastic activity in
                           vivo using modified bisphosphonates
INVENTOR(S):   Frangioni, John V.
PATENT ASSIGNEE(S):   Beth Israel Deaconess Medical Center, USA
SOURCE: PCT Int. Appl., 45 pp.
                           CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

     PATENT NO.   KIND   DATE   APPLICATION NO.   DATE
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     WO 2002038190   A2   20020516   WO 2001-US51312   20011029 <--
     WO 2002038190   A3   20020829

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   AU 2002036683        A5    20020521    AU 2002-36683           20011029 <--
   EP 1341557           A2    20030910    EP 2001-986230          20011029 <--
     R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
        IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
   US 2004028611        A1    20040212    US 2003-424572          20040212 <--
   US 6869593           B2    20050322
PRIORITY APPLN. INFO.:                     US 2000-244020P    P   20001027 <--
                                           WO 2001-US51312    W   20011029 <--
OTHER SOURCE(S):         MARPAT 136:366118
IT   424821-77-2P
     RL: ARG (Analytical reagent use); BSU (Biological study, unclassified);
     PKT (Pharmacokinetics); PRP (Properties); SPN (Synthetic preparation);
     ANST (Analytical study); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (Pam 78; nonisotopic detection of osteoblastic activity in vivo using
        modified bisphosphonates)
RN   424821-77-2   HCAPLUS
CN   3H-Indolium, 2-[2-[3-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-
     2H-indol-2-ylidene]ethylidene]-2-[4-[3-[(3-hydroxy-3,3-
     diphosphonopropyl)amino]-3-oxopropyl]phenoxy]-1-cyclohexen-1-yl]ethenyl]-
     3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-, inner salt, pentasodium salt (9CI)
     (CA INDEX NAME)
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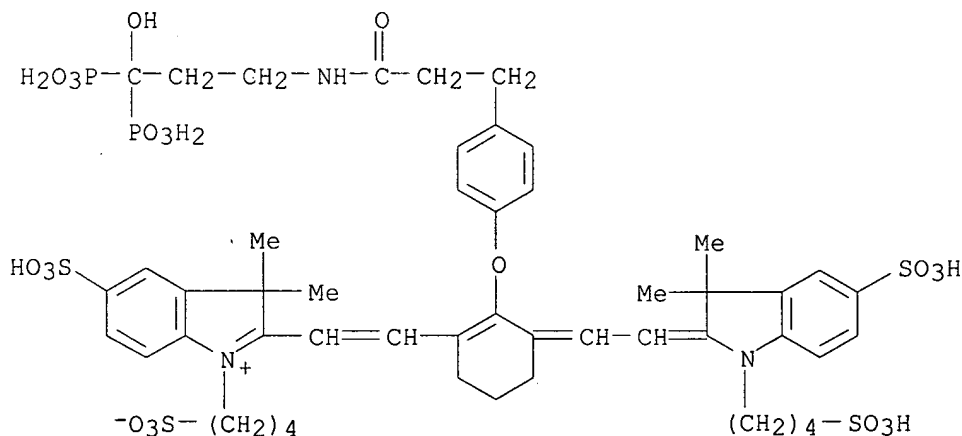

●5   Na

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IT   398142-13-7
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (nonisotopic detection of osteoblastic activity in vivo using modified
        bisphosphonates)
RN   398142-13-7   HCAPLUS
CN   3H-Indolium, 2-[2-[3-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-
     2H-indol-2-ylidene]ethylidene]-2-[4-[3-[(2,5-dioxo-1-pyrrolidinyl)oxy]-3-
     oxopropyl]phenoxy]-1-cyclohexen-1-yl]ethenyl]-3,3-dimethyl-5-sulfo-1-(4-
     sulfobutyl)-, inner salt, trisodium salt (9CI)   (CA INDEX NAME)
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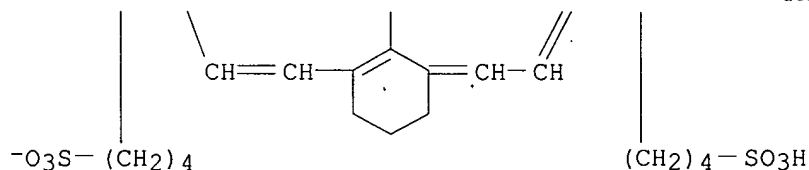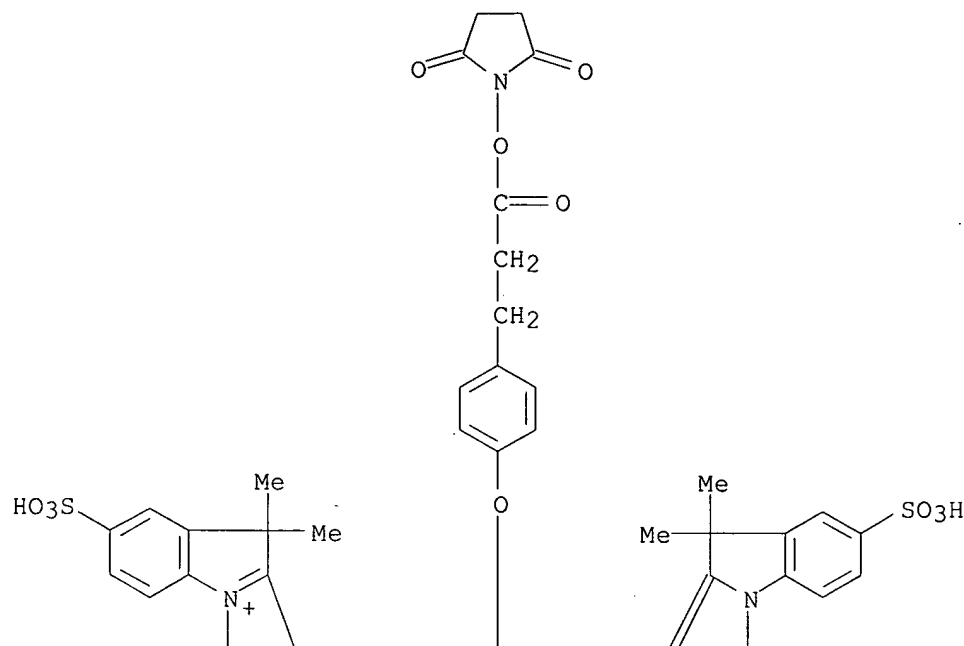
●3 Na

L32 ANSWER 8 OF 13 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:314766 HCAPLUS
DOCUMENT NUMBER: 136:321680
TITLE: Indole and benzoindole derivatives as minimally
                         invasive physiological function monitoring agents
INVENTOR(S):   Achilefu, Samuel; Rajagopalan, Raghavan; Dorshow,
                         Richard B.; Bugaj, Joseph E.
PATENT ASSIGNEE(S):   Mallinckrodt Inc., USA
SOURCE: PCT Int. Appl., 60 pp.
                         CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

    PATENT NO.   KIND   DATE   APPLICATION NO.   DATE
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    WO 2002032421   A1   20020425   WO 2001-US31719   20011005 <--

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WO 2002032421        C1      20020906
    W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
        CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR,
        HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT,
        LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU,
        SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN,
        YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
    RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
        DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,
        BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
US 6733744          B1    20040511   US 2000-688946         20001016
CA 2425701          AA    20020425   CA 2001-2425701        20011005 <--
AU 2002013100       A5    20020429   AU 2002-13100          20011005 <--
EP 1326602          A1    20030716   EP 2001-981460         20011005 <--
    R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
        IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
JP 2004526669       T2    20040902   JP 2002-535659         20011005 <--
PRIORITY APPLN. INFO.:               US 2000-688946    A    20001016 <--
                                     WO 2001-US31719   W    20011005 <--
OTHER SOURCE(S):        MARPAT 136:321680
IT   415727-03-6
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
         (indole and benzoindole derivs. as minimally invasive physiol. function
         monitoring agents)
RN   415727-03-6  HCAPLUS
CN   D-Glucose, 6-O-[[2-[2-[3,3-bis(hydroxymethyl)-5,7-disulfo-1-(3-
     sulfopropyl)-3H-indolium-2-yl]ethenyl]-6-[[1,3-dihydro-3,3-
     bis(hydroxymethyl)-5,7-disulfo-1-(3-sulfopropyl)-2H-indol-2-
     ylidene]ethylidene]-1,4-cyclohexadien-1-yl]methyl]-, inner salt (9CI)  (CA
     INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.
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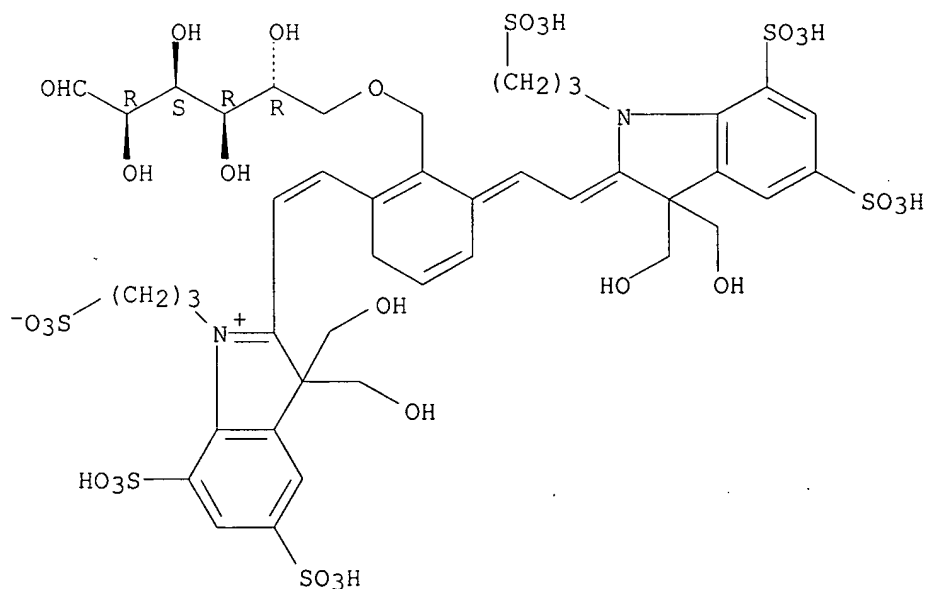


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IT   415727-04-7P
     RL: SPN (Synthetic preparation); PREP (Preparation)
         (indole and benzoindole derivs. as minimally invasive physiol. function
         monitoring agents)
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RN   415727-04-7 HCAPLUS
CN   D-Glucose, 6-O-[5-[3,3-bis(hydroxymethyl)-5-sulfo-1-(4-sulfobutyl)-3H-
      indolium-2-yl]-2-[3-[1,3-dihydro-3,3-bis(hydroxymethyl)-5-sulfo-1-(4-
      sulfobutyl)-2H-indol-2-ylidene]-1-propenyl]-2,4-pentadienyl]-, inner salt
      (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.
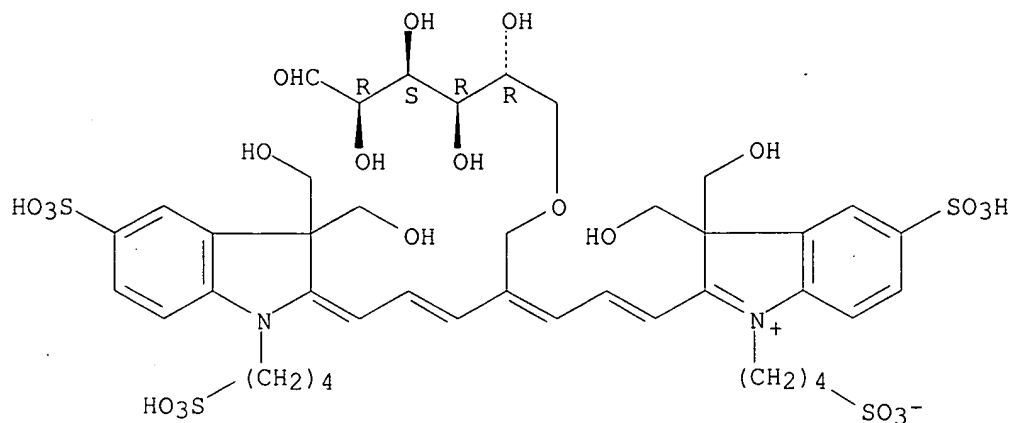
REFERENCE COUNT: 3   THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS
                                 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 9 OF 13 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2001:909860 HCAPLUS
DOCUMENT NUMBER: 136:163487
TITLE: In vivo near-infrared fluorescence imaging of
                          osteoblastic activity
AUTHOR(S):   Zaheer, Atif; Lenkinski, Robert E.; Mahmood, Ashfaq;
                          Jones, Alun G.; Cantley, Lewis C.; Frangioni, John V.
CORPORATE SOURCE: Department of Radiology, Beth Israel Deaconess Medical
                          Center, Boston, MA, 02215, USA
SOURCE: Nature Biotechnology (2001), 19(12),
                          1148-1154
                          CODEN: NABIF9; ISSN: 1087-0156
PUBLISHER: Nature America Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
IT   **397858-89-8P**
     RL: ARU (Analytical role, unclassified); SPN (Synthetic preparation); ANST
     (Analytical study); PREP (Preparation)
        (in vivo near-IR fluorescence imaging of osteoblastic activity)
RN   397858-89-8 HCAPLUS
CN   3H-Indolium, 2-[2-[3-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-
     2H-indol-2-ylidene]ethylidene]-2-[4-[3-[(3-hydroxy-3,3-
     diphosphonopropyl)amino]-3-oxopropyl]phenoxy]-1-cyclohexen-1-yl]ethenyl]-
     3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-, inner salt, heptasodium salt (9CI)
        (CA INDEX NAME)

● 7 Na

$$\text{CH}=\text{CH}-\text{C}=\text{C}=\text{CH}-\text{CH}$$

$$^-\text{O}_3\text{S}-(\text{CH}_2)_4 \qquad\qquad (\text{CH}_2)_4-\text{SO}_3\text{H}$$
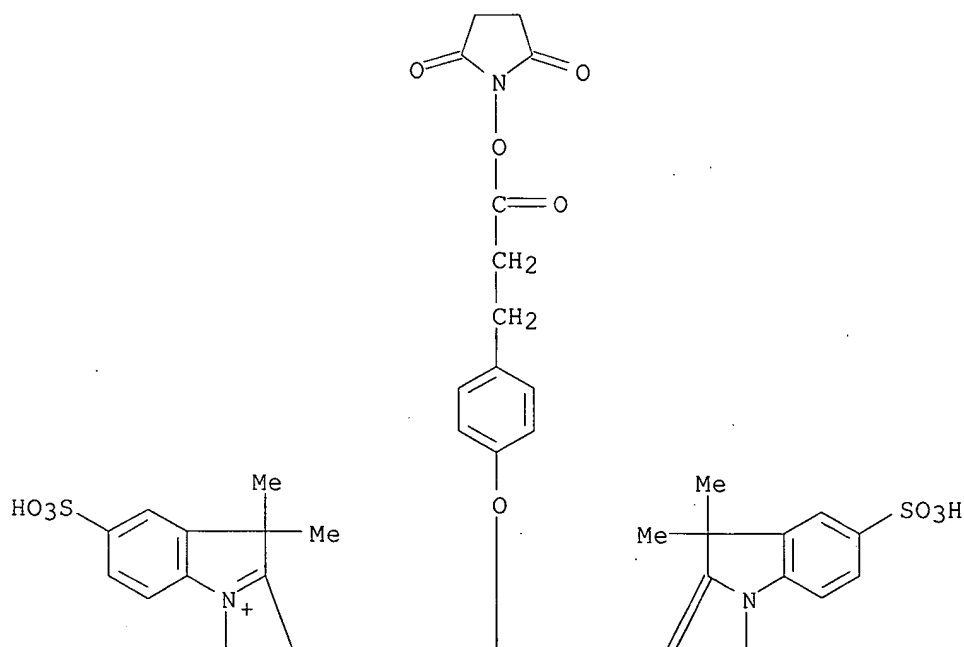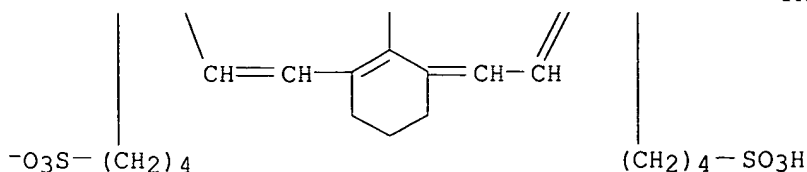
● 3 Na

REFERENCE COUNT: 39   THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS
                                  RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 10 OF 13 USPATFULL on STN
ACCESSION NUMBER: 2004:328247 USPATFULL
TITLE: Hydrophilic, thiol-reactive cyanine dyes and conjugates
                          thereof with biomolecules for fluorescence diagnosis
INVENTOR(S):   Licha, Kai, Falkensee, GERMANY, FEDERAL REPUBLIC OF
                          Perlitz, Christin, Berlin, GERMANY, FEDERAL REPUBLIC OF

                              NUMBER   KIND   DATE
                          ----------------- ------ --------
PATENT INFORMATION: US 2004260072   A1   20041223
APPLICATION INFO.:   US 2004-762582   A1   20040123   (10)

                              NUMBER   DATE
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PRIORITY INFORMATION: DE 2003-10302787 20030124   <--
                          US 2003-443197P   20030129 (60)
DOCUMENT TYPE: Utility
FILE SEGMENT: APPLICATION
LEGAL REPRESENTATIVE: MILLEN, WHITE, ZELANO & BRANIGAN, P.C., 2200 CLARENDON
                          BLVD., SUITE 1400, ARLINGTON, VA, 22201
NUMBER OF CLAIMS: 34
EXEMPLARY CLAIM: 1
LINE COUNT: 1227
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT   731862-91-2P 731862-98-9P 731863-01-7P
     731863-04-0P 731863-05-1P 731863-06-2P
     731863-08-4P 731863-09-5P 731863-10-8P
     (manufacture of hydrophilic, thiol-reactive cyanine dyes and conjugates
     thereof with biomols. for fluorescence diagnosis)
RN   731862-91-2 USPATFULL
CN   3H-Indolium, 2-[4-(2-carboxyethyl)-7-[1,3-dihydro-3,3-dimethyl-5-sulfo-1-
     (2-sulfoethyl)-2H-indol-2-ylidene]-1,3,5-heptatrienyl]-3,3-dimethyl-5-
     sulfo-1-(2-sulfoethyl)-, inner salt, trisodium salt (9CI) (CA INDEX
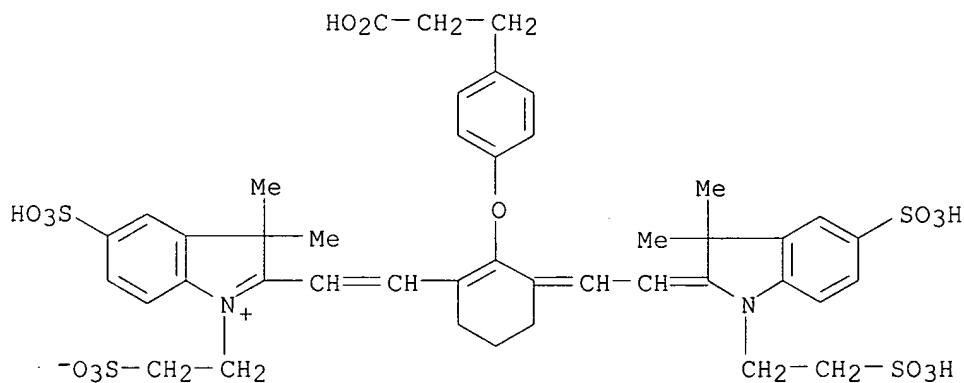   NAME)

$$\text{HO}_3\text{S}\ \ \overset{\text{Me}}{\underset{\ }{\diagup}}\ \ \text{Me} \qquad \text{HO}_2\text{C}-\text{CH}_2-\text{CH}_2 \qquad \text{Me}\ \ \overset{\text{Me}}{\underset{\ }{\diagdown}}\ \ \text{SO}_3\text{H}$$

$$\text{CH}=\text{CH}-\text{CH}=\text{C}-\text{CH}=\text{CH}-\text{CH}$$

$$^-\text{O}_3\text{S}-\text{CH}_2-\text{CH}_2 \qquad\qquad \text{CH}_2-\text{CH}_2-\text{SO}_3\text{H}$$
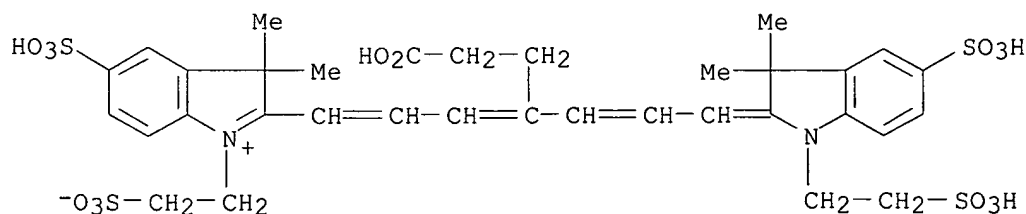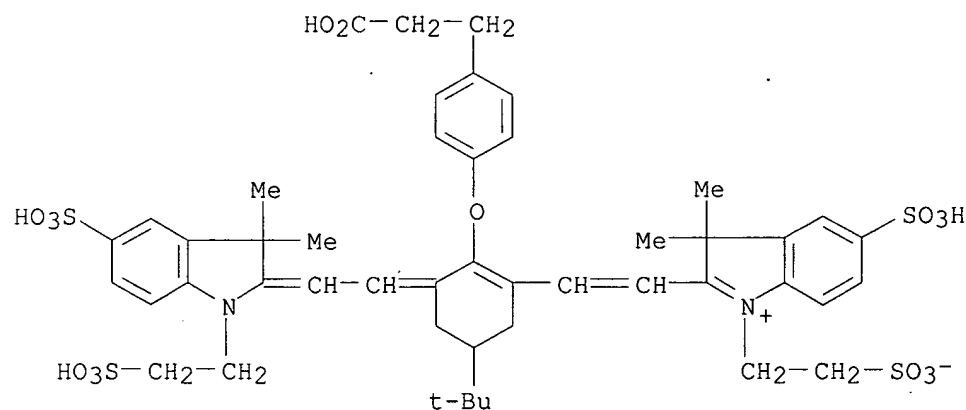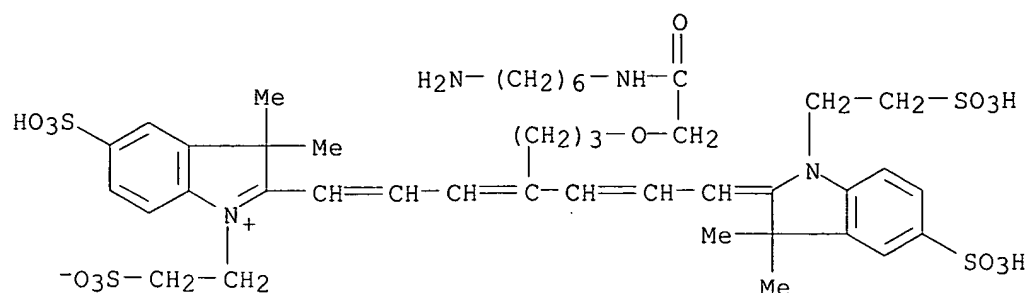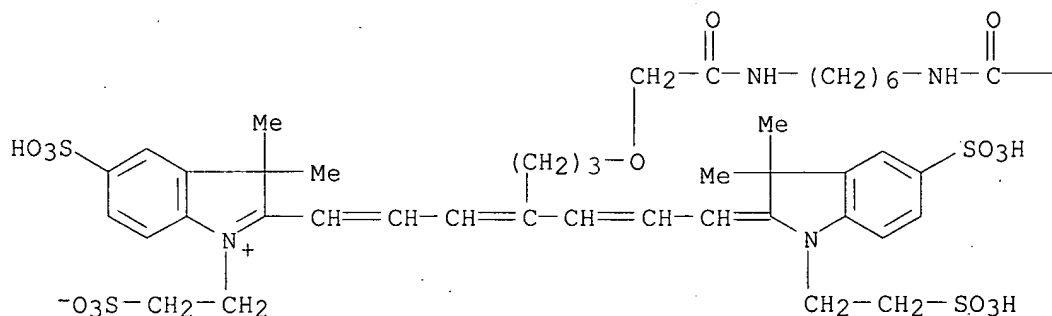
● 3 Na

RN   731862-98-9   USPATFULL
CN   3H-Indolium, 2-[8-carboxy-4-[3-[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-
      sulfoethyl)-2H-indol-2-ylidene]-1-propenyl]-1,3-octadienyl]-3,3-dimethyl-
      5-sulfo-1-(2-sulfoethyl)-, inner salt, trisodium salt (9CI)   (CA INDEX
      NAME)
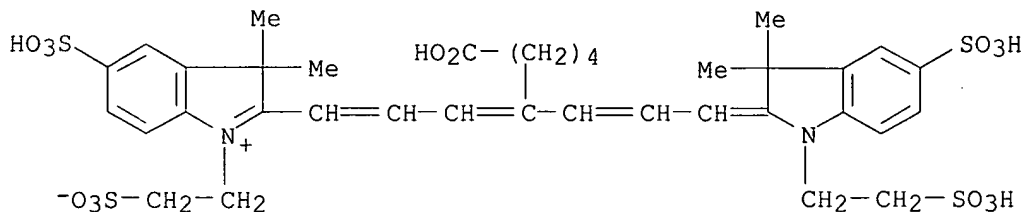
●3   Na

RN   731863-01-7   USPATFULL
CN   3H-Indolium, 2-[10-carboxy-4-[3-[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-
      sulfoethyl)-2H-indol-2-ylidene]-1-propenyl]-1,3-decadienyl]-3,3-dimethyl-
      5-sulfo-1-(2-sulfoethyl)-, inner salt, trisodium salt (9CI)   (CA INDEX
      NAME)
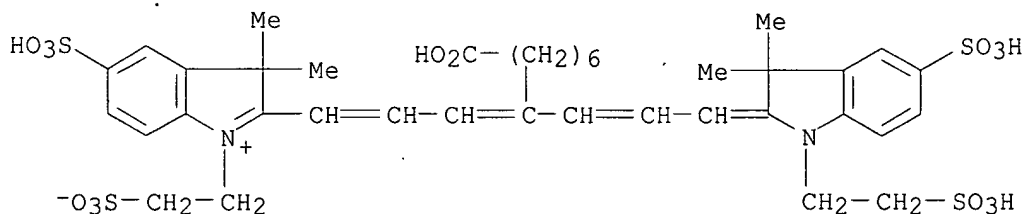
●3   Na

RN   731863-04-0   USPATFULL
CN   3H-Indolium, 2-[4-[3-(2-carboxyethoxy)propyl]-7-[1,3-dihydro-3,3-dimethyl-
      5-sulfo-1-(2-sulfoethyl)-2H-indol-2-ylidene]-1,3,5-heptatrienyl]-3,3-
      dimethyl-5-sulfo-1-(2-sulfoethyl)-, inner salt, trisodium salt (9CI)
      (CA INDEX NAME)
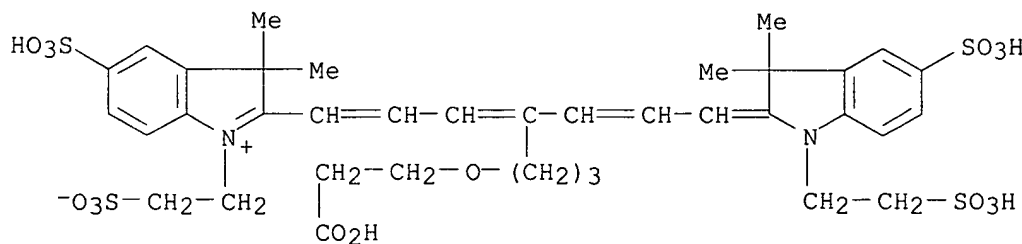
●3   Na

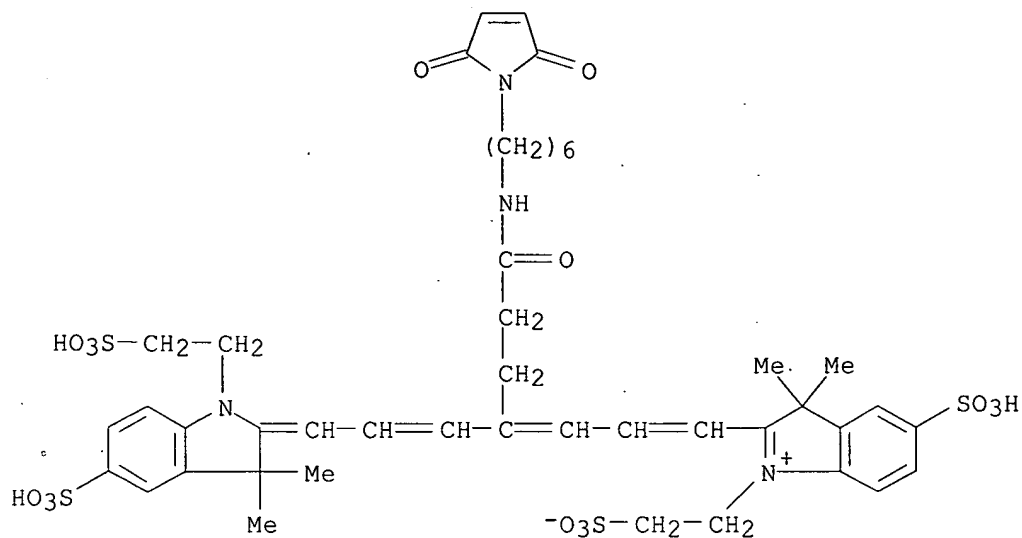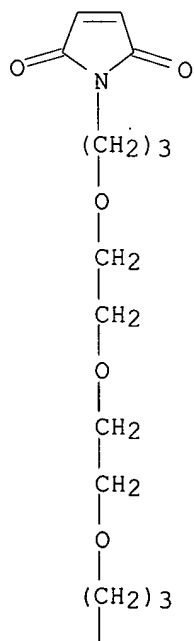RN   731863-05-1   USPATFULL
CN   3H-Indolium, 2-[2-[2-chloro-3-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-
      sulfoethyl)-2H-indol-2-ylidene]ethylidene]-1-cyclohexen-1-yl]ethenyl]-
      3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-, inner salt, trisodium salt (9CI)
         (CA INDEX NAME)

HO3S   Me   Cl   Me   SO3H
                          Me   Me   Me
                   CH=CH   =CH-CH
              N+   N
   -O3S-CH2-CH2   CH2-CH2-SO3H
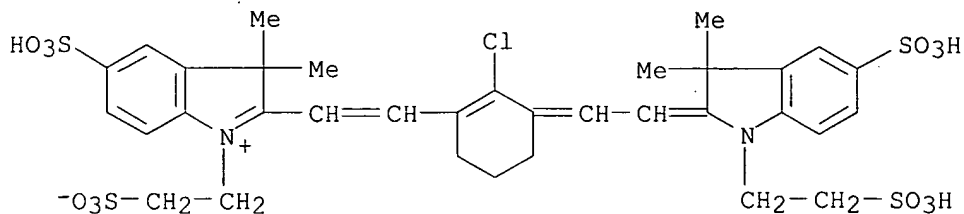
● 3 Na

RN   731863-06-2   USPATFULL
CN   3H-Indolium, 2-[2-[2-[4-(2-carboxyethyl)phenoxy]-3-[[1,3-dihydro-3,3-
      dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-indol-2-ylidene]ethylidene]-1-
      cyclohexen-1-yl]ethenyl]-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-, inner
      salt, trisodium salt (9CI)   (CA INDEX NAME)

                   HO2C-CH2-CH2

                            O

HO3S   Me   Me   SO3H
                          Me   Me   Me
                   CH=CH   =CH-CH
              N+   N
   -O3S-CH2-CH2   CH2-CH2-SO3H

● 3   Na

RN   731863-08-4   USPATFULL
CN   3H-Indolium, 2-[2-[2-chloro-3-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-
      sulfoethyl)-2H-indol-2-ylidene]ethylidene]-5-(1,1-dimethylethyl)-1-
      cyclohexen-1-yl]ethenyl]-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-, inner
      salt, trisodium salt (9CI)   (CA INDEX NAME)
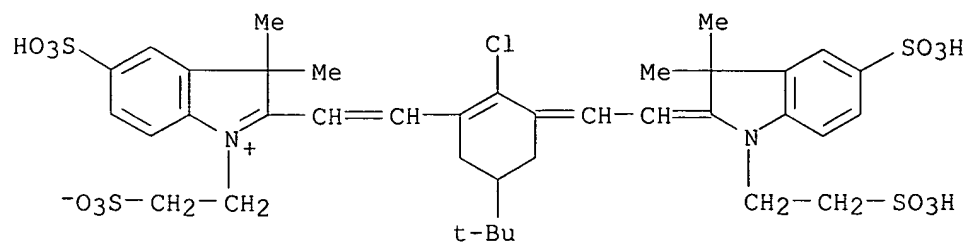
●3 Na

RN   731863-09-5 USPATFULL
CN   3H-Indolium, 2-[2-[2-[4-(2-carboxyethyl)phenoxy]-3-[[1,3-dihydro-3,3-
      dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-indol-2-ylidene]ethylidene]-5-(1,1-
      dimethylethyl)-1-cyclohexen-1-yl]ethenyl]-3,3-dimethyl-5-sulfo-1-(2-
      sulfoethyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)

●3 Na

RN   731863-10-8 USPATFULL
CN   3H-Indolium, 2-[4-[3-[2-[[(6-aminohexyl)amino]-2-oxoethoxy]propyl]-7-[1,3-
      dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-indol-2-ylidene]-1,3,5-
      heptatrienyl]-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-, inner salt,
      trisodium salt (9CI) (CA INDEX NAME)

●3 Na

PAGE 1-A

●3 Na

PAGE 1-B

— CH2Br

indol-2-ylidene]-4-[3-[[2-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-
yl)ethyl]amino]-3-oxopropyl]-1,3,5-heptatrienyl]-3,3-dimethyl-5-sulfo-1-
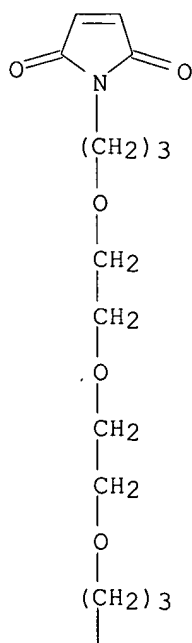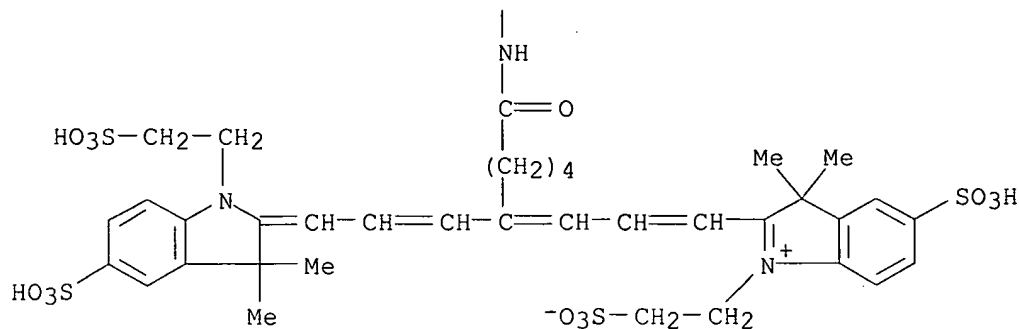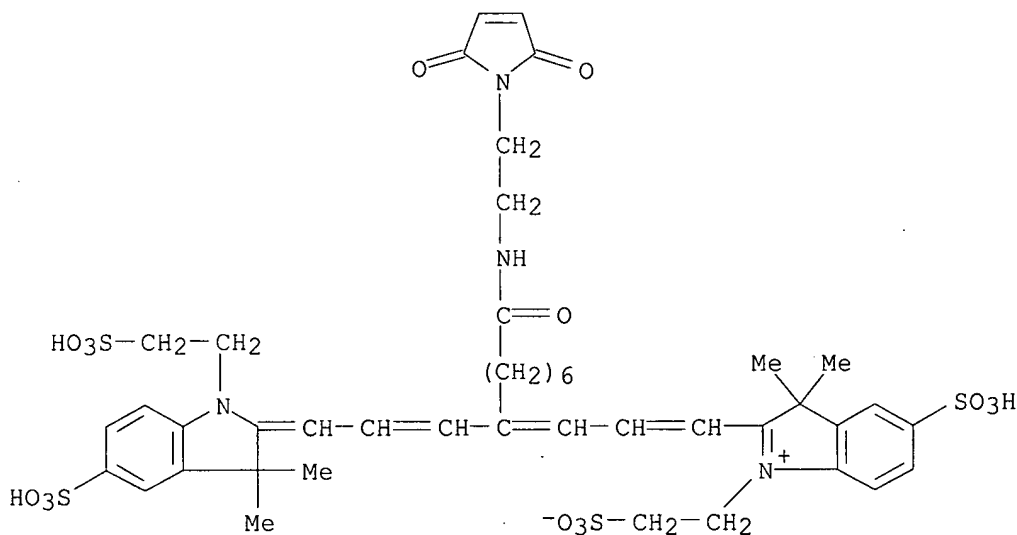(2-sulfoethyl)-, inner salt, trisodium salt (9CI)   (CA INDEX NAME)

●3   Na

RN   731862-72-9   USPATFULL
CN   3H-Indolium, 2-[7-[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-
      indol-2-ylidene]-4-[3-[[6-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-
      yl)hexyl]amino]-3-oxopropyl]-1,3,5-heptatrienyl]-3,3-dimethyl-5-sulfo-1-
      (2-sulfoethyl)-, inner salt, trisodium salt (9CI)   (CA INDEX NAME)
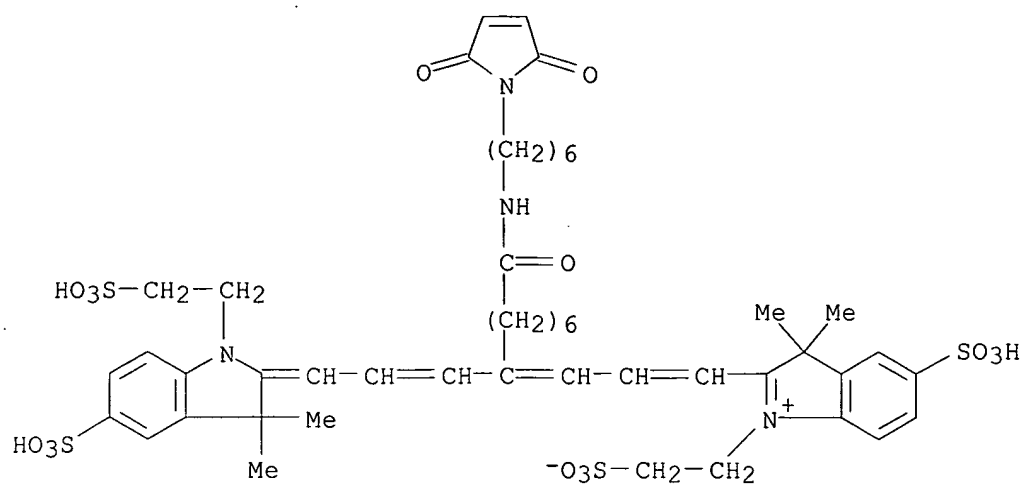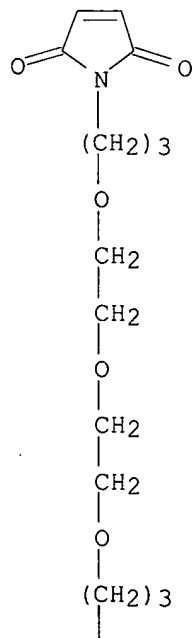
●3 Na

RN   731862-73-0 USPATFULL
CN   3H-Indolium, 2-[4-[3-[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-
     indol-2-ylidene]-1-propenyl]-21-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)-7-
     oxo-12,15,18-trioxa-8-azaheneicosa-1,3-dien-1-yl]-3,3-dimethyl-5-sulfo-1-
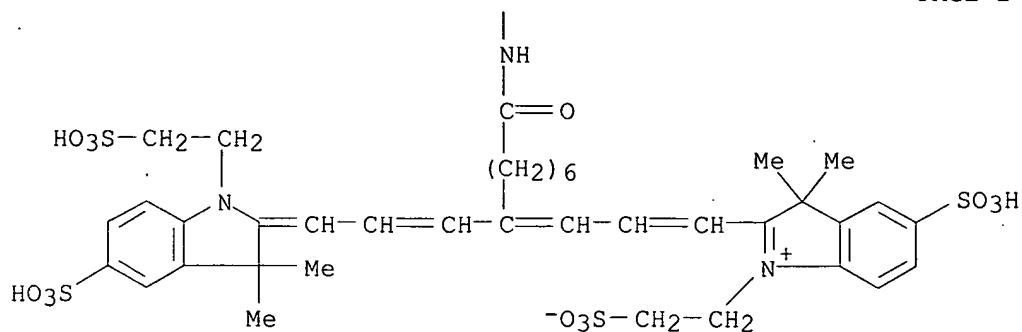   (2-sulfoethyl)-, inner salt, trisodium salt (9CI)   (CA INDEX NAME)
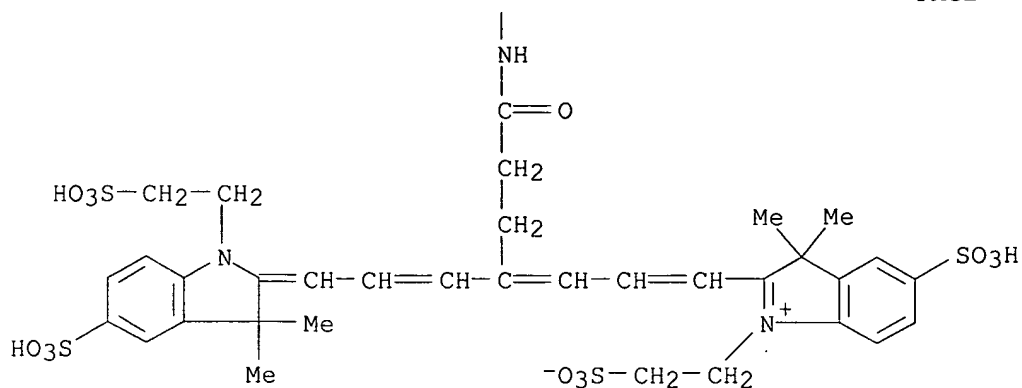
●3 Na

RN   731862-74-1   USPATFULL
CN   3H-Indolium, 2-[4-[3-[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-
      indol-2-ylidene]-1-propenyl]-9-[[2-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-
      yl)ethyl]amino]-9-oxo-1,3-nonadienyl]-3,3-dimethyl-5-sulfo-1-(2-
      sulfoethyl)-, inner salt, trisodium salt (9CI)   (CA INDEX NAME)
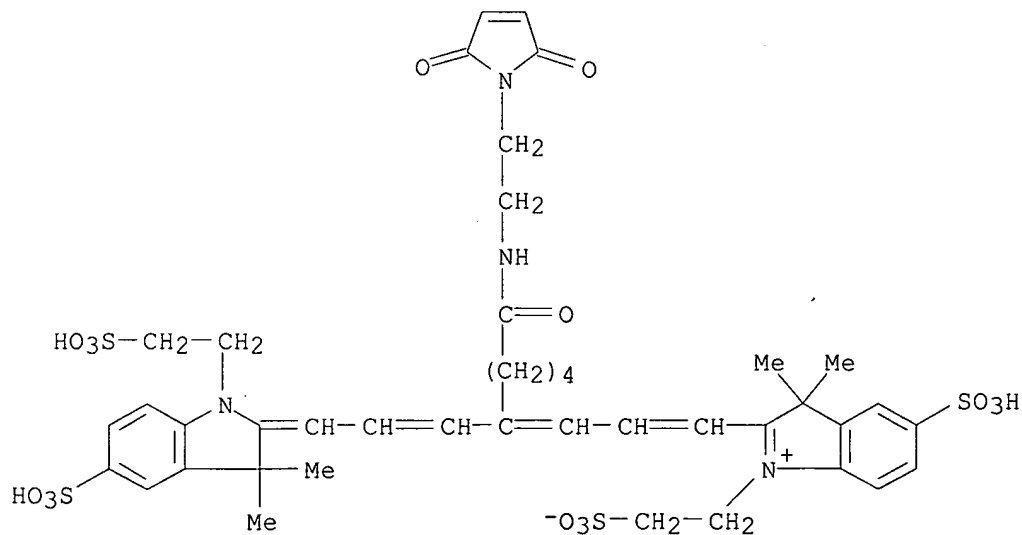
●3 Na

RN   731862-75-2   USPATFULL
CN   3H-Indolium, 2-[4-[3-[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-
      indol-2-ylidene]-1-propenyl]-9-[[6-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-
      yl)hexyl]amino]-9-oxo-1,3-nonadienyl]-3,3-dimethyl-5-sulfo-1-(2-
      sulfoethyl)-, inner salt, trisodium salt (9CI)   (CA INDEX NAME)
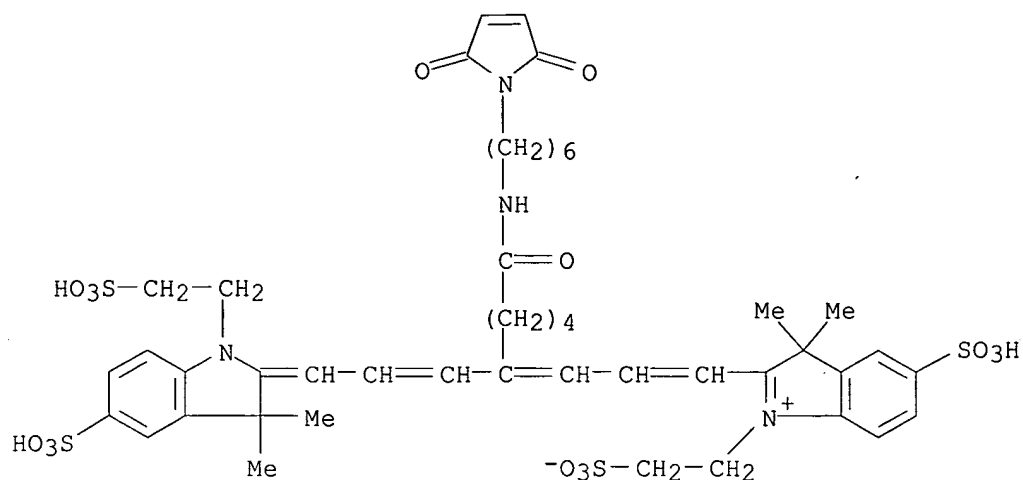
●3 Na

RN   731862-76-3 USPATFULL
CN   3H-Indolium, 2-[4-[3-[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-
      indol-2-ylidene]-1-propenyl]-23-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)-9-
      oxo-14,17,20-trioxa-10-azatricosa-1,3-dien-1-yl]-3,3-dimethyl-5-sulfo-1-
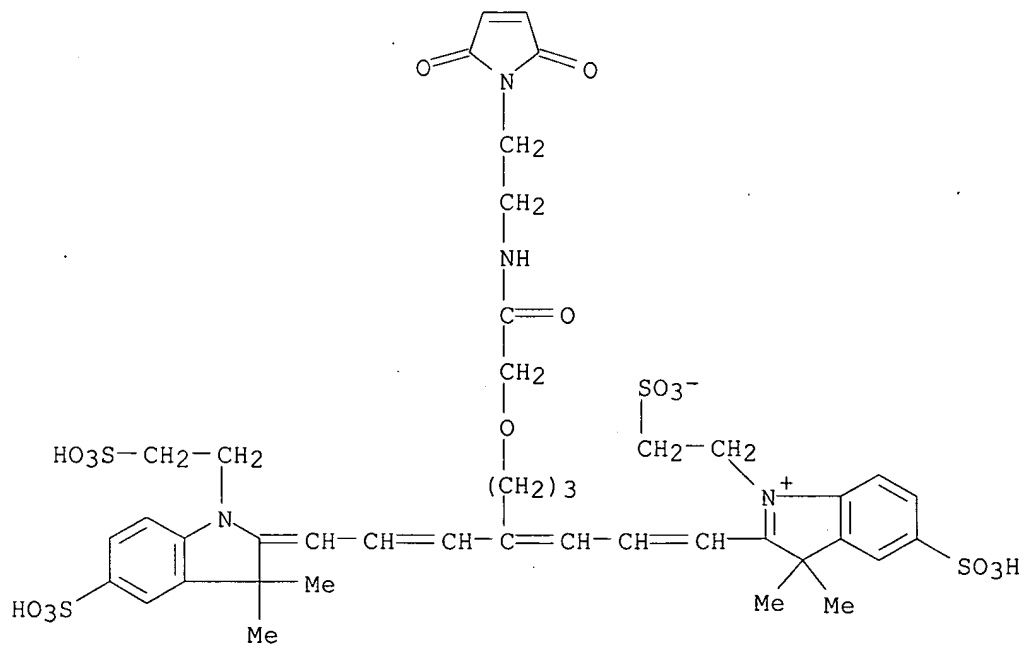   (2-sulfoethyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)

PAGE 1-A

HO3S—CH2—CH2

NH
|
C=O
|
(CH2)4
|

Me   Me

SO3H

CH=CH—CH=C—CH—CH=CH

HO3S

Me
Me

⁻O3S—CH2—CH2

N⁺

●3 Na

RN   731862-77-4 USPATFULL
CN   3H-Indolium, 2-[4-[3-[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-
     indol-2-ylidene]-1-propenyl]-11-[[2-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-
     yl)ethyl]amino]-11-oxo-1,3-undecadienyl]-3,3-dimethyl-5-sulfo-1-(2-
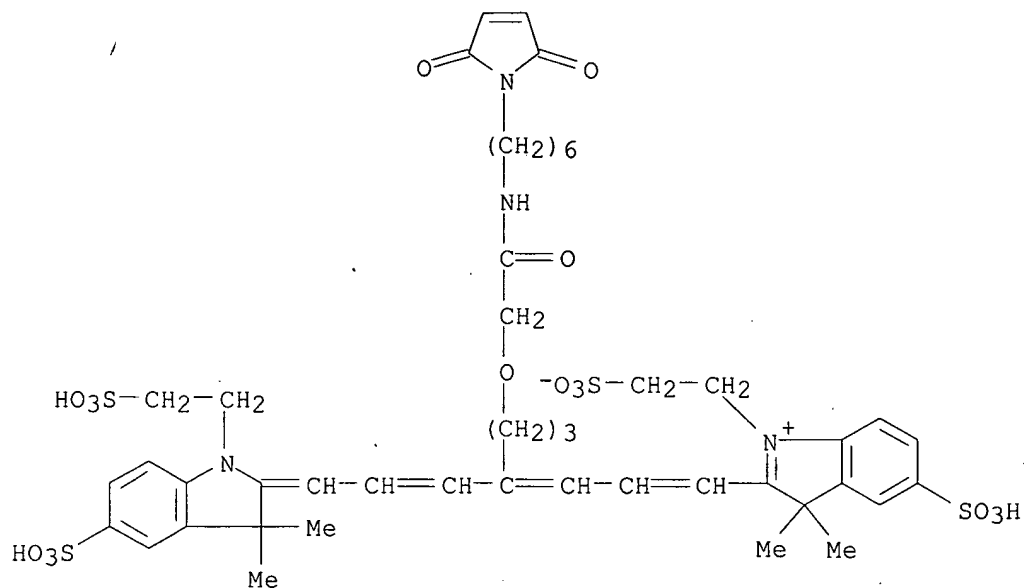   sulfoethyl)-, inner salt, trisodium salt (9CI)   (CA INDEX NAME)

O   N   O

CH2
|
CH2
|
NH
|
C=O
|
(CH2)6
|

HO3S—CH2—CH2

Me   Me

SO3H

CH—CH=CH—C=CH—CH=CH

HO3S

Me
Me

⁻O3S—CH2—CH2

N⁺

●3 Na

RN   731862-78-5 USPATFULL
CN   3H-Indolium, 2-[4-[3-[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-
     indol-2-ylidene]-1-propenyl]-11-[[6-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-
     yl)hexyl]amino]-11-oxo-1,3-undecadienyl]-3,3-dimethyl-5-sulfo-1-(2-
     sulfoethyl)-, inner salt, trisodium salt (9CI)   (CA INDEX NAME)

●3 Na

PAGE 1-A

● 3 Na

RN   731862-80-9   USPATFULL
CN   3H-Indolium, 2-[7-[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-
      indol-2-ylidene]-4-[3-[2-[[2-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-
      yl)ethyl]amino]-2-oxoethoxy]propyl]-1,3,5-heptatrienyl]-3,3-dimethyl-5-
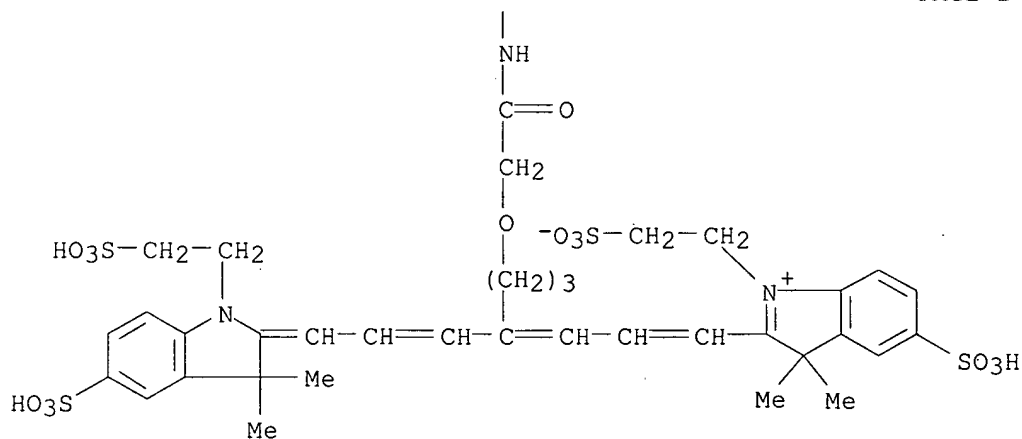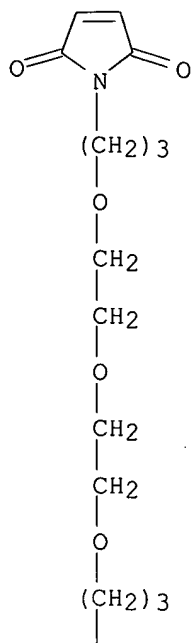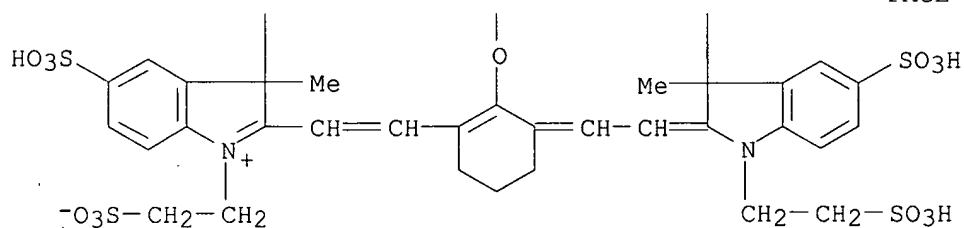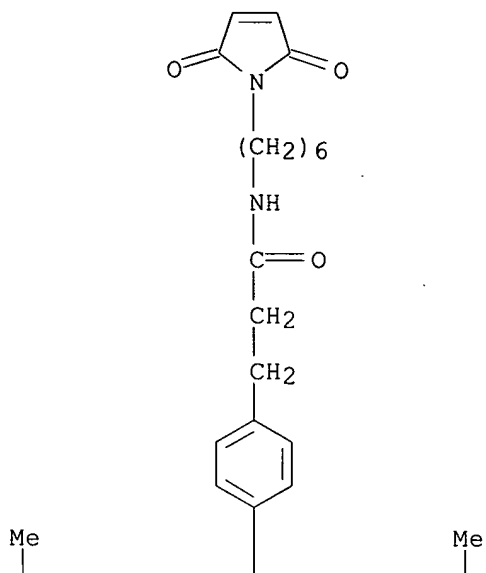   sulfo-1-(2-sulfoethyl)-, inner salt, trisodium salt (9CI)   (CA INDEX
      NAME)

● 3 Na

RN   731862-81-0   USPATFULL
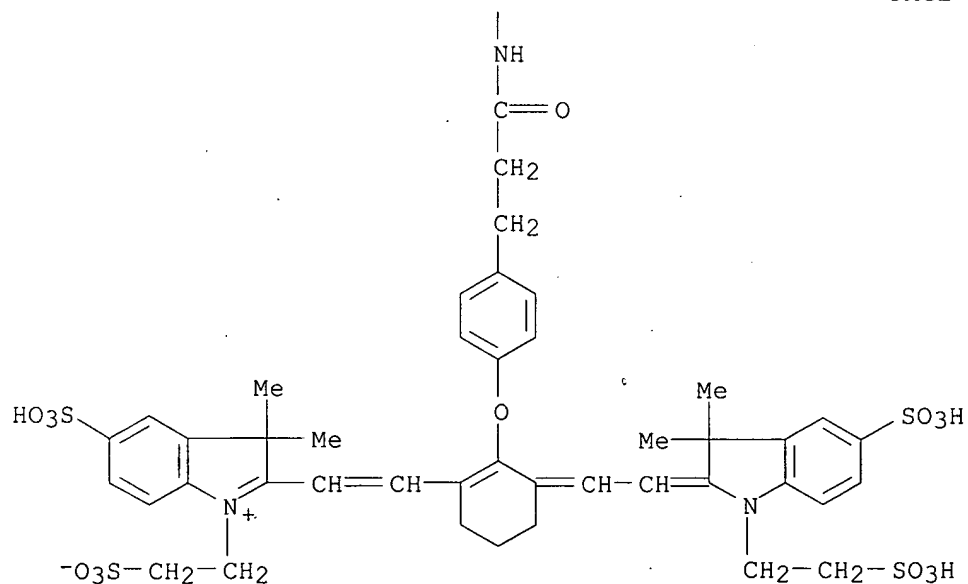CN   3H-Indolium, 2-[7-[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-
      indol-2-ylidene]-4-[3-[2-[[6-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-

yl)hexyl]amino]-2-oxoethoxy]propyl]-1,3,5-heptatrienyl]-3,3-dimethyl-5-
sulfo-1-(2-sulfoethyl)-, inner salt, trisodium salt (9CI) (CA INDEX
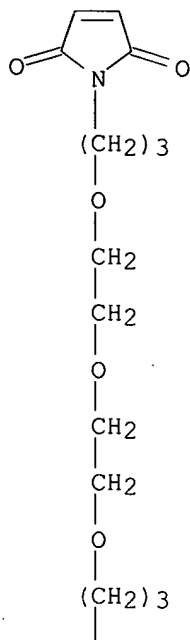NAME)

●3 Na

RN   731862-82-1 USPATFULL
CN   3H-Indolium, 2-[4-[3-[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-
     indol-2-ylidene]-1-propenyl]-24-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)-
     10-oxo-8,15,18,21-tetraoxa-11-azatetracosa-1,3-dien-1-yl]-3,3-dimethyl-5-
     sulfo-1-(2-sulfoethyl)-, inner salt, trisodium salt (9CI) (CA INDEX
     NAME)

$(CH_2)_3$

O

CH_2

CH_2

O

CH_2

CH_2

O

$(CH_2)_3$

● 3 Na

RN   731862-83-2   USPATFULL
CN   3H-Indolium, 2-[2-[3-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-
     2H-indol-2-ylidene]ethylidene]-2-[4-[3-[[2-(2,5-dihydro-2,5-dioxo-1H-
     pyrrol-1-yl)ethyl]amino]-3-oxopropyl]phenoxy]-1-cyclohexen-1-yl]ethenyl]-
     3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-, inner salt, trisodium salt (9CI)
     (CA INDEX NAME)

●3 Na

RN   731862-84-3 USPATFULL
CN   3H-Indolium, 2-[2-[3-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-
      2H-indol-2-ylidene]ethylidene]-2-[4-[3-[[6-(2,5-dihydro-2,5-dioxo-1H-
      pyrrol-1-yl)hexyl]amino]-3-oxopropyl]phenoxy]-1-cyclohexen-1-yl]ethenyl]-
      3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-, inner salt, trisodium salt (9CI)
      (CA INDEX NAME)

● 3 Na

RN   731862-85-4   USPATFULL
CN   3H-Indolium, 2-[2-[3-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-
     2H-indol-2-ylidene]ethylidene]-2-[4-[17-(2,5-dihydro-2,5-dioxo-1H-pyrrol-
     1-yl)-3-oxo-8,11,14-trioxa-4-azaheptadec-1-yl]phenoxy]-1-cyclohexen-1-
     yl]ethenyl]-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-, inner salt,
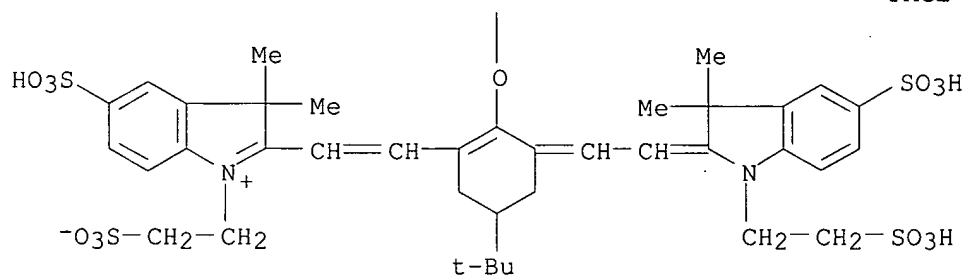   trisodium salt (9CI) (CA INDEX NAME)

O
N
O

(CH₂)₃

O

CH₂

CH₂

O

CH₂

CH₂

O

(CH₂)₃

NH

C═O

CH₂

CH₂

O

HO3S

Me

Me

CH═CH

CH─CH

Me

Me

SO3H

N+

N

⁻O3S─CH₂─CH₂

CH₂─CH₂─SO3H

●3 Na

RN   731862-86-5 USPATFULL
CN   3H-Indolium, 2-[2-[3-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-
      2H-indol-2-ylidene]ethylidene]-2-[4-[3-[[2-(2,5-dihydro-2,5-dioxo-1H-
      pyrrol-1-yl)ethyl]amino]-3-oxopropyl]phenoxy]-5-(1,1-dimethylethyl)-1-

cyclohexen-1-yl]ethenyl]-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-, inner
salt, trisodium salt (9CI) (CA INDEX NAME)
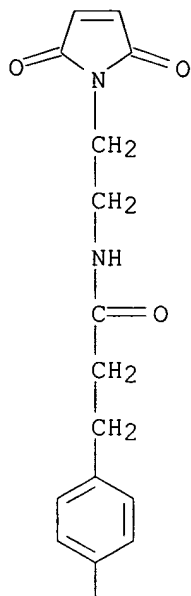
●3 Na

RN   731862-88-7 USPATFULL
CN   3H-Indolium, 2-[4-[3-[[3-[(bromoacetyl)amino]propyl]amino]-3-oxopropyl]-7-
      [1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-indol-2-ylidene]-
      1,3,5-heptatrienyl]-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-, inner salt,
      trisodium salt (9CI) (CA INDEX NAME)
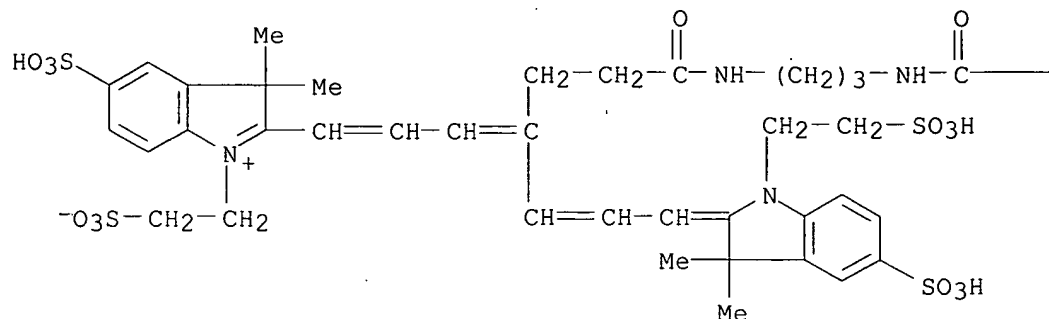
●3 Na

— CH2Br

L32   ANSWER 11 OF 13   USPATFULL on STN
ACCESSION NUMBER: 2004:292756 USPATFULL
TITLE: Modified PSMA ligands and uses related thereto
INVENTOR(S):   Frangioni, John V., Wayland, MA, UNITED STATES
PATENT ASSIGNEE(S):   Beth Israel Deaconess Medical Center, Boston, MA (U.S.
                         corporation)

                         NUMBER   KIND   DATE
                         ---------------- ------ --------
PATENT INFORMATION: US 2004229845   A1   20041118
APPLICATION INFO.:   US 2004-869790   A1   20040616 (10)
RELATED APPLN. INFO.:   Continuation of Ser. No. US 2002-71890, filed on 7 Feb
                         2002, PENDING

                         NUMBER   DATE
                         ------------------ --------
PRIORITY INFORMATION: US 2001-267055P   20010207 (60)   <--
DOCUMENT TYPE: Utility
FILE SEGMENT: APPLICATION
LEGAL REPRESENTATIVE: ROPES & GRAY LLP, ONE INTERNATIONAL PLACE, BOSTON, MA,
                         02110-2624
NUMBER OF CLAIMS: 66
EXEMPLARY CLAIM: 1
NUMBER OF DRAWINGS: 11 Drawing Page(s)
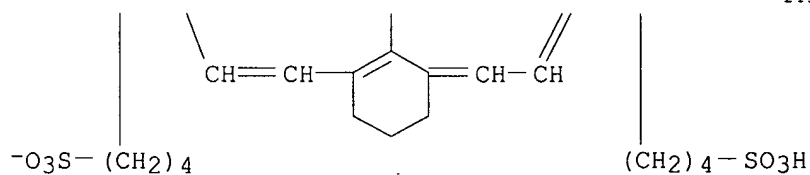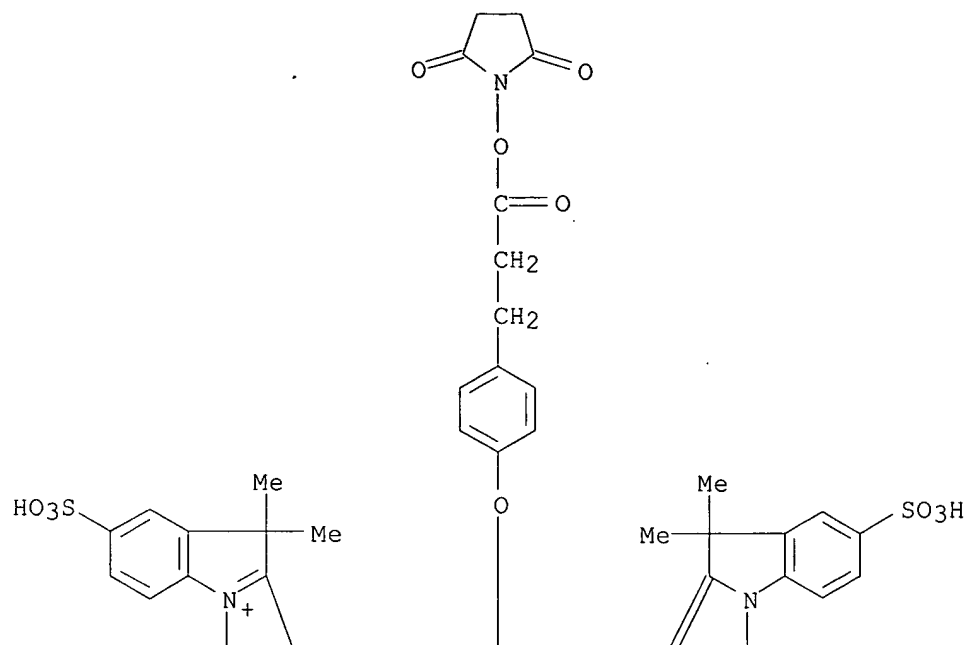LINE COUNT: 1759
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT 398142-13-7, IRDye78
       (modified PSMA ligands for diagnosis and treatment of prostate cancer)
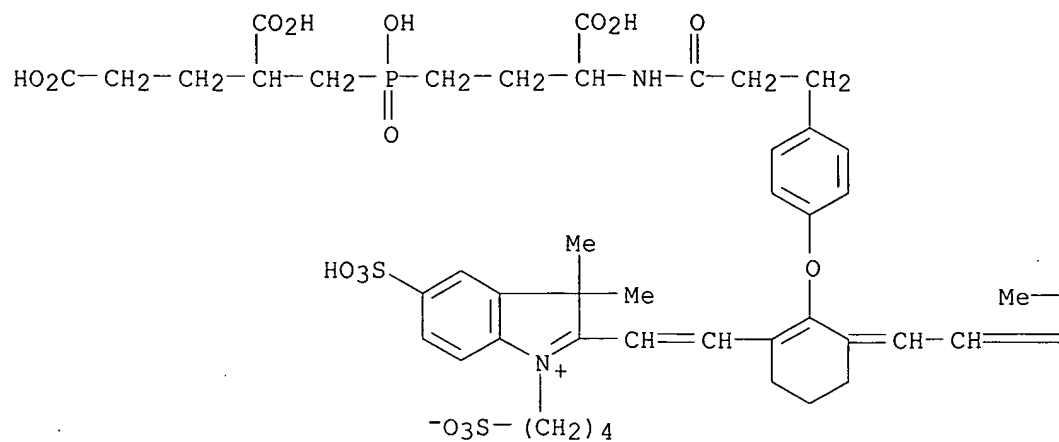RN   398142-13-7 USPATFULL
CN   3H-Indolium, 2-[2-[3-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-
     2H-indol-2-ylidene]ethylidene]-2-[4-[3-[(2,5-dioxo-1-pyrrolidinyl)oxy]-3-
     oxopropyl]phenoxy]-1-cyclohexen-1-yl]ethenyl]-3,3-dimethyl-5-sulfo-1-(4-
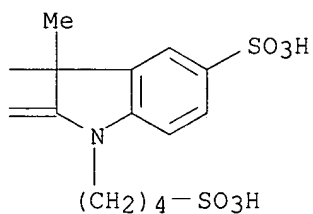   sulfobutyl)-, inner salt, trisodium salt (9CI)   (CA INDEX NAME)

● 3 Na

IT **477808-85-8 477808-86-9**
      (modified PSMA ligands for diagnosis and treatment of prostate cancer)
RN   477808-85-8 USPATFULL
CN   3H-Indolium, 2-[2-[2-[4-[3-[[1-carboxy-3-[(2,4-
      dicarboxybutyl)hydroxyphosphinyl]propyl]amino]-3-oxopropyl]phenoxy]-3-
      [[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-2H-indol-2-
      ylidene]ethylidene]-1-cyclohexen-1-yl]ethenyl]-3,3-dimethyl-5-sulfo-1-(4-
   sulfobutyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)

●3   Na

RN   477808-86-9   USPATFULL
CN   L-Glutamic acid, N-[3-[4-[[6-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(4-
     sulfobutyl)-2H-indol-2-ylidene]ethylidene]-2-[2-[3,3-dimethyl-5-sulfo-1-
     (4-sulfobutyl)-3H-indolium-2-yl]ethenyl]-1-cyclohexen-1-yl]oxy]phenyl]-1-
     oxopropyl]-L-β-aspartyl-, inner salt, trisodium salt (9CI)   (CA
     INDEX NAME)

     Absolute stereochemistry.
     Double bond geometry unknown.
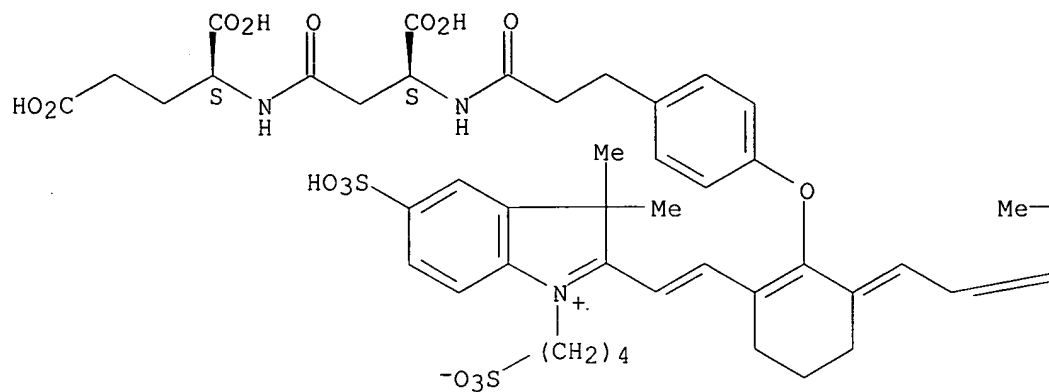
● 3 Na
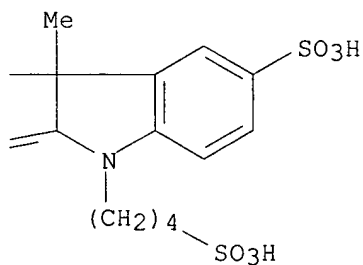
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L32   ANSWER 12 OF 13    USPATFULL on STN
ACCESSION NUMBER:        2004:145051  USPATFULL
TITLE:                   MODIFIED PSMA LIGANDS AND USES RELATED THERETO
INVENTOR(S):             Frangioni, John V., Wayland, MA, UNITED STATES

                         NUMBER          KIND     DATE
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PATENT INFORMATION:      US 2004110723    A1      20040610
                         US 6875886       B2      20050405
APPLICATION INFO.:       US 2002-71890    A1      20020207   (10)

                         NUMBER           DATE
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PRIORITY INFORMATION:    US 2001-267055P  20010207 (60)              <--
DOCUMENT TYPE:           Utility
FILE SEGMENT:            APPLICATION
LEGAL REPRESENTATIVE:    ROPES & GRAY LLP, ONE INTERNATIONAL PLACE, BOSTON, MA,
                         02110-2624
NUMBER OF CLAIMS:        66
EXEMPLARY CLAIM:         1
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NUMBER OF DRAWINGS: 11 Drawing Page(s)
LINE COUNT: 1757
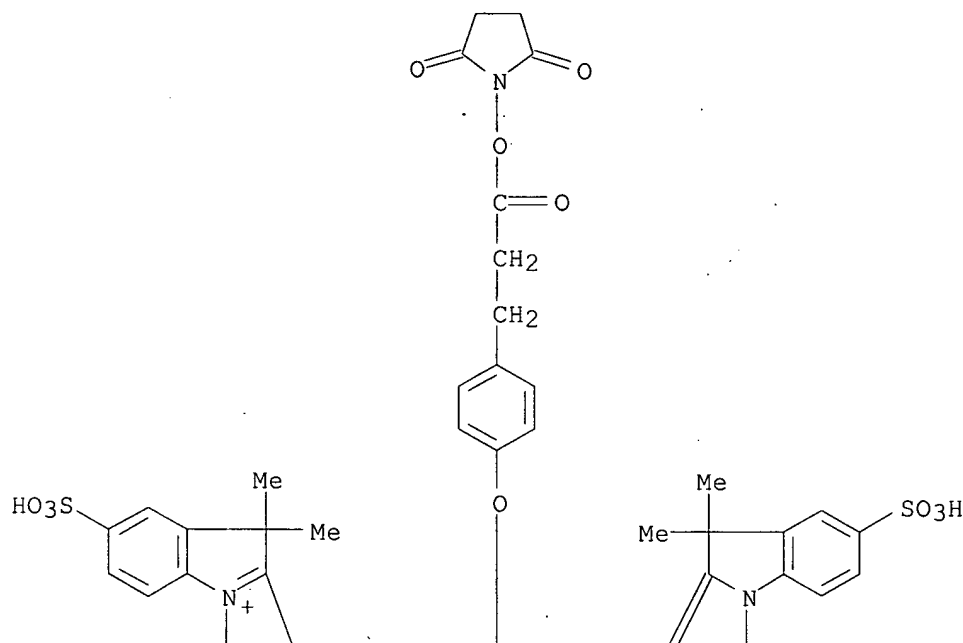CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **398142-13-7**, IRDye78
        (modified PSMA ligands for diagnosis and treatment of prostate cancer)
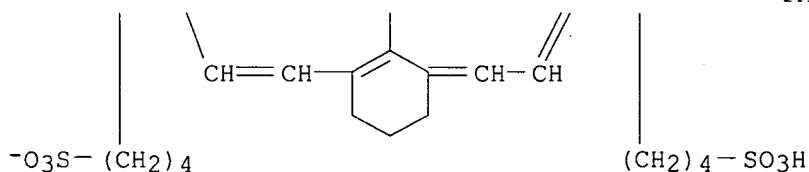RN   398142-13-7 USPATFULL
CN   3H-Indolium, 2-[2-[3-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-
      2H-indol-2-ylidene]ethylidene]-2-[4-[3-[(2,5-dioxo-1-pyrrolidinyl)oxy]-3-
      oxopropyl]phenoxy]-1-cyclohexen-1-yl]ethenyl]-3,3-dimethyl-5-sulfo-1-(4-
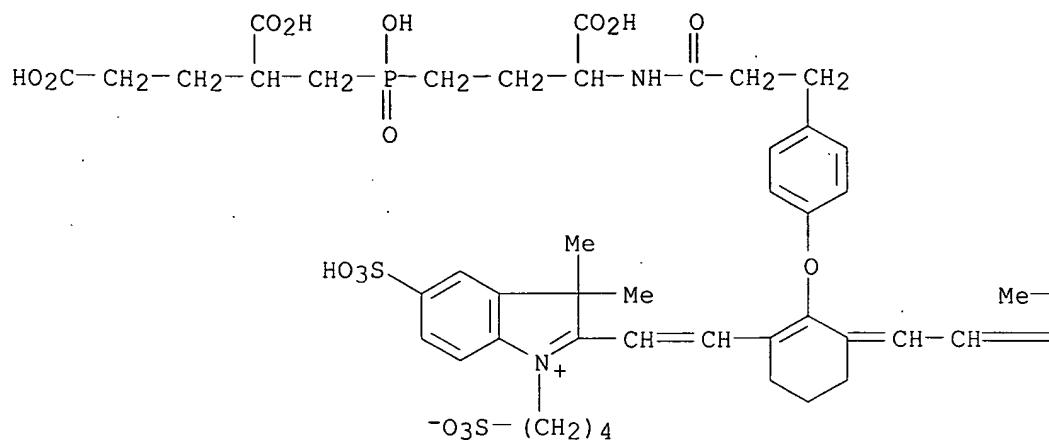   sulfobutyl)-, inner salt, trisodium salt (9CI)   (CA INDEX NAME)

IT **477808-85-8 477808-86-9**
        (modified PSMA ligands for diagnosis and treatment of prostate cancer)
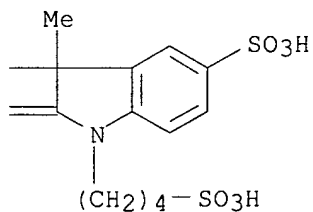RN   477808-85-8 USPATFULL
CN   3H-Indolium, 2-[2-[2-[4-[3-[[1-carboxy-3-[(2,4-
      dicarboxybutyl)hydroxyphosphinyl]propyl]amino]-3-oxopropyl]phenoxy]-3-
      [[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-2H-indol-2-
      ylidene]ethylidene]-1-cyclohexen-1-yl]ethenyl]-3,3-dimethyl-5-sulfo-1-(4-
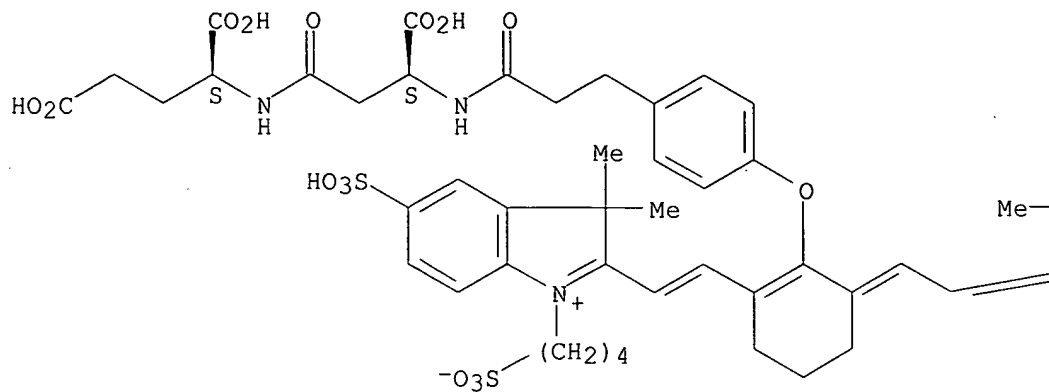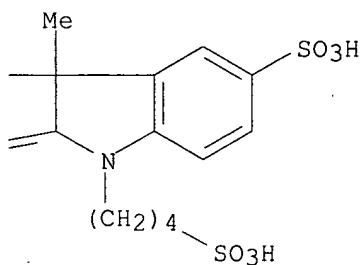   sulfobutyl)-, inner salt, trisodium salt (9CI)   (CA INDEX NAME)

RN   477808-86-9 USPATFULL
CN   L-Glutamic acid, N-[3-[4-[[6-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(4-
      sulfobutyl)-2H-indol-2-ylidene]ethylidene]-2-[2-[3,3-dimethyl-5-sulfo-1-
      (4-sulfobutyl)-3H-indolium-2-yl]ethenyl]-1-cyclohexen-1-yl]oxy]phenyl]-1-
      oxopropyl]-L-β-aspartyl-, inner salt, trisodium salt (9CI)   (CA
      INDEX NAME)

      Absolute stereochemistry.
      Double bond geometry unknown.

●3 Na

L32 ANSWER 13 OF 13   USPATFULL on STN
ACCESSION NUMBER: 2004:38075 USPATFULL
TITLE: Non-isotopic detection of osteoblastic activity in vivo
                         using modified bisphosphonates
INVENTOR(S):   Frangioni, John V., Wayland, MA, UNITED STATES
PATENT ASSIGNEE(S):   Beth Israel Deaconess Medical Center, of the entire
                         inerst. (U.S. corporation)

                              NUMBER   KIND   DATE
                         ---------------- ------ --------
PATENT INFORMATION: US 2004028611   A1   20040212
                         US 6869593   B2   20050322
APPLICATION INFO.:   US 2003-424572   A1   20030425   (10)
RELATED APPLN. INFO.:   Continuation of Ser. No. WO 2001-US51312, filed on 29
                         Oct 2001, PENDING

                              NUMBER   DATE
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PRIORITY INFORMATION: US 2000-244020P   20001027 (60)   <--
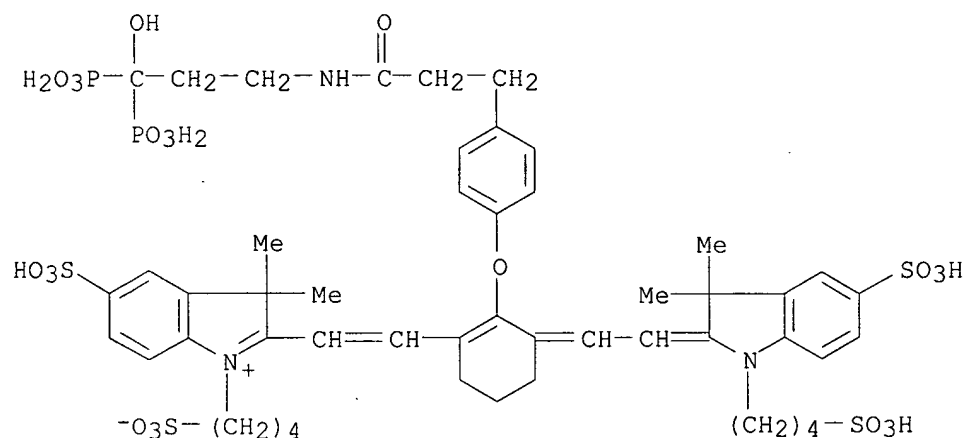DOCUMENT TYPE: Utility

IT   424821-77-2P
        (Pam 78; nonisotopic detection of osteoblastic activity in vivo using
        modified bisphosphonates)
RN   424821-77-2   USPATFULL
CN   3H-Indolium, 2-[2-[3-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-
     2H-indol-2-ylidene]ethylidene]-2-[4-[3-[(3-hydroxy-3,3-
     diphosphonopropyl)amino]-3-oxopropyl]phenoxy]-1-cyclohexen-1-yl]ethenyl]-
     3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-, inner salt, pentasodium salt
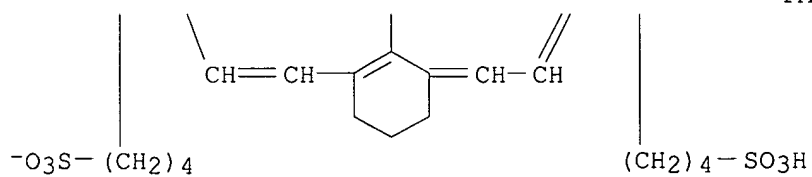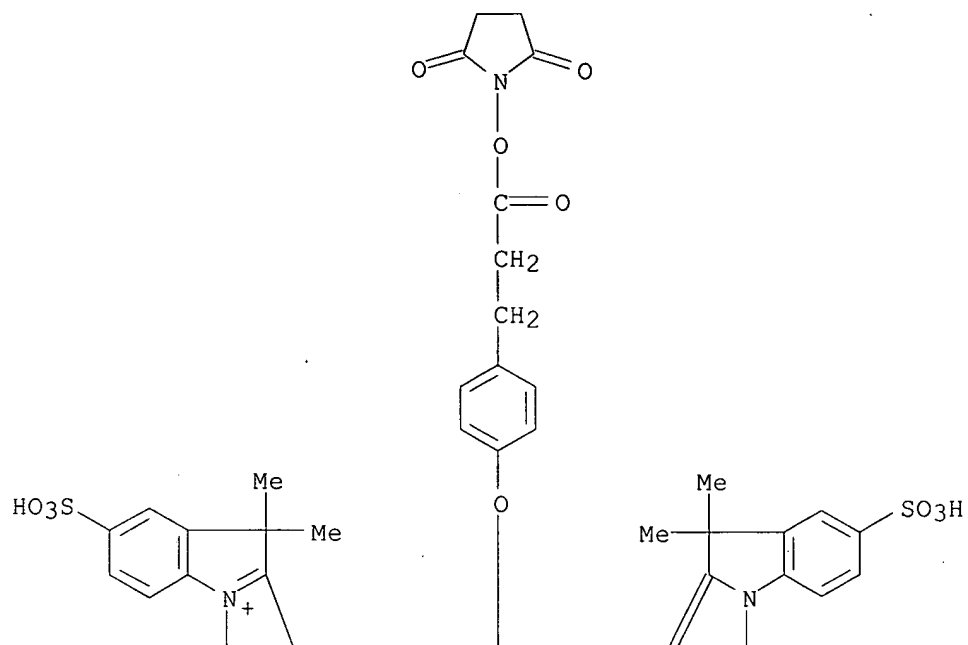   (9CI) (CA INDEX NAME)

IT   398142-13-7
        (nonisotopic detection of osteoblastic activity in vivo using modified
        bisphosphonates)
RN   398142-13-7   USPATFULL
CN   3H-Indolium, 2-[2-[3-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-
     2H-indol-2-ylidene]ethylidene]-2-[4-[3-[(2,5-dioxo-1-pyrrolidinyl)oxy]-3-
     oxopropyl]phenoxy]-1-cyclohexen-1-yl]ethenyl]-3,3-dimethyl-5-sulfo-1-(4-
     sulfobutyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)

●3 Na